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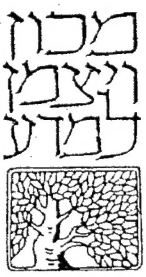

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Proceedings of the Research Workshop

of the Israel Science Foundation

on

Multiscale Phenomena, Modelling and Computation

March 2-7, 1997, Neptune Hotel, Eilat, Israel.

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Research Workshop of the Israel Science Foundation

Multiscale Phenomena, Modelling and Computation

Neptune Hotel, Eilat, Israel

2–7 March, 1997

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- *The Racah Institute of Physics at the Hebrew University of Jerusalem*
- *Universität Hamburg, Germany*

Acknowledgment. We wish to thank the United States Air Force European Office of Aerospace Research and Development for its contribution to the success of this workshop. We also thank Silicon Graphics Computer Systems, Ltd., Israel, for loaning us their workstations for the conference terminal room.

Scientists at work in the conference terminal room

Contents

Scientific Background

The nature of the interactions between different scales of phenomena in a complex system has recently become the focus of interest in an increasingly wider range of scientific fields. This interest originated independently in theoretical physics and in computational mathematics.

The emergence of macroscopic complex phenomena in systems composed of many simple microscopic elements, and, inversely, the construction of microscopic laws to explain macroscopic measurements, have been at the center stage of physics for more than a century. In particular, a systematic procedure for advancing the system description from fine to increasingly coarser scales — the renormalization group method — has been developed, mainly in the context of particle physics.

At the same time, with the introduction of computer simulations into increasingly larger and more complex systems, it has become clear that major bottlenecks in scientific computations (in physics, chemistry and engineering) can be overcome by organizing algorithms in *multiscale* (or "multiresolution" or "multilevel" or "multigrid") fashions.

The typical multiscale algorithm iteratively construct a sequence of system descriptions at a sequence of representative scales, combining local processing at each scale with various inter-scale interactions.

Usually, the evolving solution on each scale recursively dictates the *equations* (or the Hamiltonian) on coarser scales and modifies the *solution* (or configuration) on finer scales. In this way large-scale changes are effectively performed on coarse grids, based on information previously gathered from finer grids.

As a result of such multilevel interactions, the fine scales of the problem can be employed very sparingly, and sometimes only at special and/or representative small regions. Moreover, the inter-scale interactions can eliminate various kinds of difficulties, such as: slow convergence (in minimization processes, PDE solvers, etc.); critical slowing down (in statistical physics); ill-posedness (e.g., of inverse problems); large-scale attraction basin traps (in global optimization and statistical simulations); conflicts between small-scale and large-scale representations (e.g., in wave problems); numerousness of interactions (in many body problems or integral equations); the need to produce many fine-level solutions (e.g., in optimal control) or very many fine-level independent samples (in statistical physics); etc.

Also, the multiscale interactions tend to bring out the large-scale dynamics, or the macroscopic equations, of the physical system, which is often, as mentioned above, the very objective of the entire calculation. It turns out that designing multi-scale algorithms for a system based on microscopic rules and understanding the macroscopic phenomena born out of those rules are just two facets of the same endeavor. The computer programs and methods become the very expression of the scientific understanding which they helped to uncover.

The multiscale paradigm has already yielded, or showed its potential to yield, central advances in diverse disciplines, such as: theoretical physics (e.g., quantum gravity, (un-)computability of physical systems, field theories, magnetic and solid state systems, quarks and gluons, random surfaces and dynamical interfaces, spin glasses and astrophysics), computational chemistry (e.g., ab-initio quantum chemistry and molecular mechanics), engineering (fluid dynamics, structural mechanics, waves and many other fields governed by differential equations), tomography, image processing and image understanding, theory of inventive thinking, cognition and thought dynamics, economics and social planning.

The Multiscale Physicalist Paradigm might eventually develop into a framework for defining, identifying and studying the salient collective macroscopic features of complex systems in a most general context. As such it would constitute a strong conceptual and methodological unifying factor over a very wide range of scientific, technological and other domains.

This unexpected and disturbing break of established interdisciplinary borders prompted several physicists and applied mathematicians to convene in February 95 an interdisciplinary workshop in Eilat to map the scope and the objectives of the Multiscale methodology.

During the meeting, attended by 70 scientists, the integrative potential of the Multiscale paradigm became evident and the continuation of this dialog has been urged by many. The purpose of the second Eilat workshop has been to bring together again different communities of researchers interested in the methodology, derivation, exploitation, and philosophical implications of multiscale interactions.

The participants include three main groups: theoretical physicists, computational mathematicians and chemists. The physicists are mainly originating in the field theory and statistical mechanics communities, especially in the theoretical and/or simulation aspects of renormalization group, criticality and universality. Many of them have lately manifested a growing interest in the more general theory of dynamical and complex phenomena and/or in their computational aspects. The participating mathematicians represent several subcommunities which have adopted different versions of multiscale scientific computation: multigrid, multipole, hierarchical bases, wavelets, and other related areas. A group of computational chemists and material scientists represent their growing interest in multiscale methods, especially for ab-initio quantum chemistry and for molecular dynamics.

Conference Program

March 2–7, 1997

Sunday, March 2, 1997

13:00	*Registration*
19:00	*Welcome Reception*

Monday, March 3, 1997

Hour	*Place*	*Organizer*	*Title*
09:00	main	Solomon	Welcome and opening remarks
09:15	main	Solomon	Why the hell am I here?
10:00	main	Atlan	Genetics is not in the genes
10:30	*Coffee break*		
11:15	main	Brandt	Efficiency in multiscale computation
	Break		
15:30	*Coffee break*		
16:00	main		*Abstract Session* (Zenger, McWilliams, Pinn, Adi, Goldenberg, Stauffer)
17:00	main	Meyer	Spectra of Dirac operator in random matrix model
17:00	video	Zenger	Group discussion of grid adaptation
17:45	main	Trottenberg	Tutorial: basic multigrid
17:45	small	Ta'asan	One-shot methods for differential optimization
20:00	main	Brandt	Finishing morning survey
21:00	main	Stauffer	Sex and the single bit

Tuesday, March 4, 1997

Hour	*Place*	*Organizer*	*Title*
09:00	main	Kerszberg	Multiscale in biology
09:00	video	Ta'asan	Computational fluid dynamics
10:00	main	Stauffer	Multiscale relaxation
	Coffee break		
11:00	main	Mack	Renormalization group tutorial
12:00	main		*Abstract Session* (Goldenberg, Aharonov, Biham, Lidar, Fomel, Vorontsov, Lauwers, Rubin)
	Break		
14:30	main	Goldenberg	Can creativity manifest itself in computers?
15:30	main	Aharonov	The transition from quantum to classical physics from the point of view of a quantum-computationalist (& discussion)
15:30	*Coffee break*		
16:00	video	Livshits	Multigrid solution for standing wave equation
16:30	main	Cohen	Immunological homunculus
16:30	video	Fomel	Software development center. Conception of "black-hole"
17:30	main	Group	Turbulence tutorial
17:30	video	Rubin	Abrupt learning in visual perception
18:30	video	Domany	Clustering of Data
18:30	small	Group	Multigrid CFD (cont'd)
19:30	corner	Cohen Solomon Savit Kerszberg	WHAT ARE: Fundamental laws, emergent laws and models. Building a physics-biology dictionary
20:00	video	Hoffman Lauwers	M.C. simulations of biomolecule-water systems
20:10	main	Lidar	Simulating Ising spin systems on a quantum computer

Wednesday, March 5, 1997

Hour	*Place*	*Organizer*	*Title*
09:00	video	Pinn	Study on analyticity of renormalization group
09:00	small	Adi	Reductionism in children's graphic expression (DEMO)
09:00	main	Group	Fast summation of long-range forces (Glaser, Essmann, Venner, Smith, Brandt)
10:00	video	Biham	Fractals, scaling and power laws
10:30	*Coffee break*		
11:00	video	Spinks	Creativity and multilevel connectionism
11:00	main	Nitzan	Multiscale problems in molecular dynamics
11:15	main	Brandt	Multiscale molecular dynamics
12:00	main		*Abstract Session* (Sharon, Vannimenus, Janke, Savit, Popa, Meier-Schellersheim, Galam, Wieczerkowski)
13:00	main	Kerszberg	Scales in biology tutorial
14:00	video	Group	Computers and creativity (2nd discussion)
	Break		
16:00	*Conference Excursion*		

Thursday, March 6, 1997

Hour	*Place*	*Organizer*	*Title*
09:00	main	Averbuch	Wavelet tutorial
09:45–13:00	main	*WAVELET SESSION:*	
		Fischer	Numerical study of Schroedinger Eq. in a wavelet basis
		Farge	Coherent structures extraction and computation in 2D turbulence using wavelets
		Schneider	Adaptive wavelet methods for nonlinear PDEs with applications to Navier-Stokes and reaction-diffusion eq.
		Israeli/ Averbuch	Sparse solution of elliptic problems
		Averbuch	Image compression using wavelets
09:00	video	Becker	Reduced variable MD
09:00	small	Lidar	Simulating spin systems on a quantum computer
09:45	small	Smith	Interfacing models (polymers)
10:30	*Coffee break*		
11:00	video	Janke	Multicanonical multigrid and clusters simulations
12:00	video	Paul	Interfacing models (polymers)
12:30	video	Galam	Do humans behave like atoms
13:30	video	Group	Scaling in stock market (Levy, Stauffer Solomon, Biham)
	Break		
14:00	small	Group	Computer against professors: results from round 1 (10 min.)
14:30	video	Galun	Optimal multigrid algorithms for calculating thermodynamic limits
14:30	main	Wieczerkowski	Renormalized QFT from renormalization Invariance

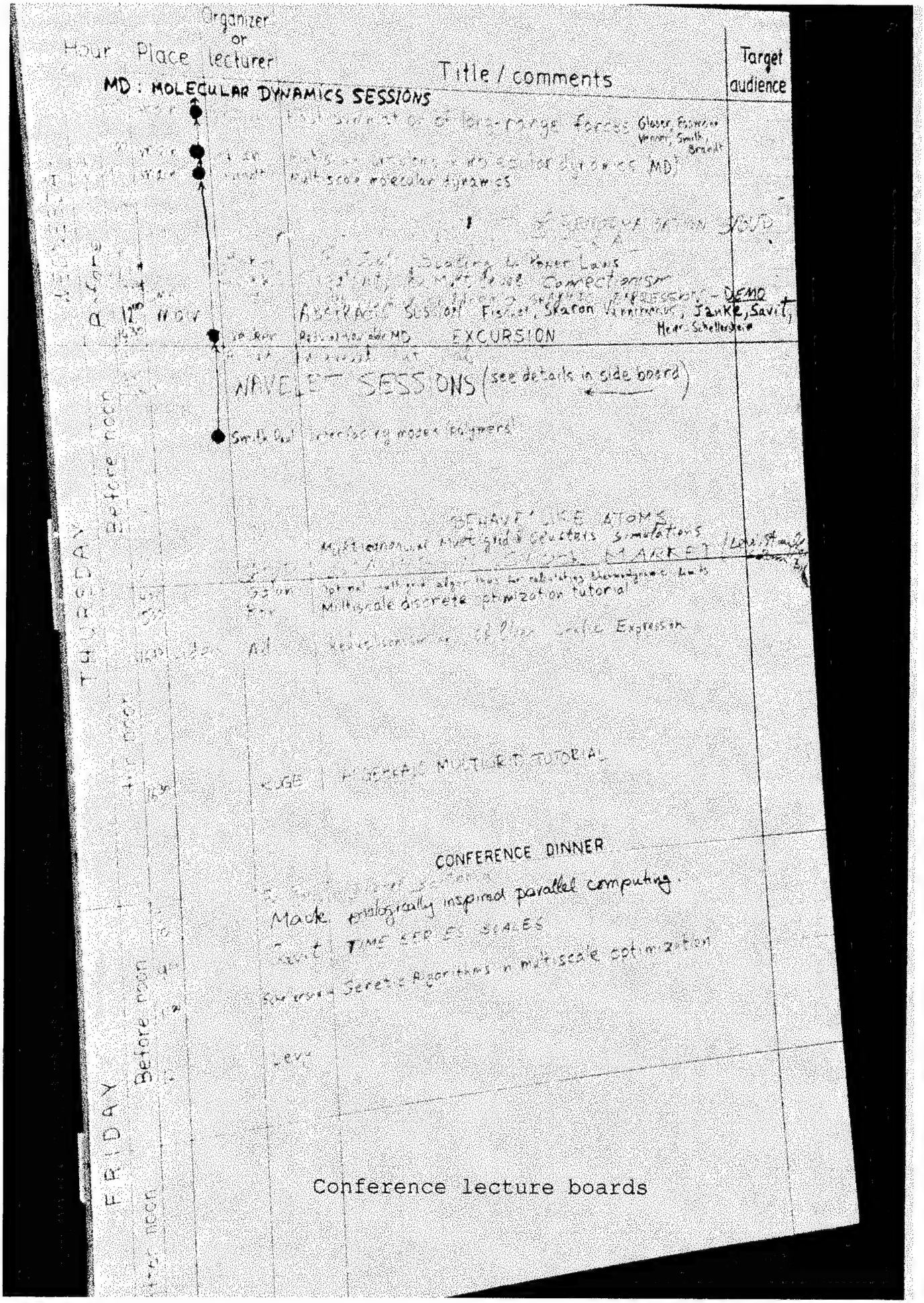
Thursday, March 6, 1997 — Cont'd

Hour	*Place*	*Organizer*	*Title*
15:30	video	Ron	Multiscale discrete optimization tutorial
15:30	main	Ruge	Algebraic multigrid tutorial
16:30	main	Ben-Jacob	Bacterial wisdom, Gödel + creative genomic web
16:30	video	Adi	Reductionism in children's graphic expression
17:30	video	Savit	Time series scales and epilepsy
20:00	*Conference Dinner*		

Friday, March 7, 1997

Hour	*Place*	*Organizer*	*Title*
09:00	main	Bai	Multiscale energy minimization in simple molecular chains
09:00–10:00	video	Group	Models in biology (Atlan, Mack Kerszberg, Solomon)
10:30	*Coffee break*		
11:00	main	Sharon	Multiscale in computer vision
14:00	*Conference bus departs for the north*		

	Hour	Place	Organizer or lecturer	Title / comments	Target audience
MONDAY Before noon	[illegible]	[illegible]	[illegible]	[illegible]	
	[illegible]	main	[illegible]	[illegible]	
	[illegible]	main	[illegible]	[illegible] is not in the [illegible]	
	[illegible]	main	[illegible]	Efficiency of multiscale computation	
After noon	16	main		ABSTRACT SESSION [illegible]	
	[illegible]	main	Meyer	Spectra of [illegible] in random matrix model	
	[illegible]	[illegible]	[illegible]	Tutorial: Basic multigrid	
	17	[illegible]	Zenger	Group discussion of grid adaptation	
				[illegible]	
	20	main	[illegible]	[illegible] survey	
				[illegible] and the Single [illegible]	
Before noon	[illegible]	main	Kurzberg	Multiscale in Biology	
			Tasan	COMPUTATIONAL FLUID DYNAMICS	
	9.00	VIDEO	[illegible]	Multiscale Relaxation	
				[illegible] Group Tutorial	
	[illegible]	main	[illegible]		
	12	main		ABSTRACT SESSION Goldenberg, [illegible], Landau, [illegible], Fomel, [illegible], [illegible]	
				[illegible]	
	15.00	[illegible]	[illegible]	[illegible] Workshop	
			[illegible]	[illegible] Development Center Conception of "Black Hole"	
After noon	16.30	Video	Fomel		
	[illegible]	main	[illegible]	[illegible] tutorial	
				CLUSTERING OF DATA	
	18.30	small	[illegible]	[illegible]	
				[illegible]	
	20	Video	[illegible]		



Conference lecture boards

Reductionism in Children's Graphic Expression

Esther Adi
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Jerusalem, Israel

Abstract

It is well known that as children start primary school they loose their motivation to draw. Is it because of internal processes or because of social influence. In a Demo we shall see several cases which I hope will shed some light on this phenomenon.

Polynomial Simulations of Decohered Quantum Computers

Dorit Aharonov[1] and *Michael Ben-Or*[2]

[1] Institutes of Physics and Computer Science
The Hebrew University, Jerusalem, Israel

[2] Institute of Computer Science, The Hebrew University, Jerusalem, Israel

Abstract

Quantum computers are now believed to be exponentially faster than classical computers. We investigate the computational power of noisy quantum computers, by presenting a Monte-Carlo simulation of these computers on a classical computer. We find that the simulation is efficient (polynomial) when the noise is larger than some critical value (this is the "classical region"), but exponential when the noise is lower than the critical value ("quantum region").

This result might have an impact on the way we understand the transition from quantum to classical physics, and can be interpreted as an indication to the fact that this transition is, in some cases, a sharp phase transition.

Fault-Tolerant Quantum Computation with Constant Error

Dorit Aharonov[1] and *Michael Ben-Or*[2]

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[2] Institute of Computer Science, The Hebrew University, Jerusalem, Israel

Abstract

In the past year many developments have taken place in the area of quantum error corrections. Recently Shor showed how to perform fault tolerant quantum computation when, η, the probability for a fault in one time step per qubit or per gate, is polylogarithmically small. This paper closes the gap and shows how to perform fault tolerant quantum computation when the error probability, η, is smaller than some constant threshold, η_0. The cost is polylogarithmic in time and space, and no measurements are used during the quantum computation. The same result is shown also for quantum circuits which operate on nearest neighbors only.

To achieve this noise resistance, we use concatenated quantum error correcting codes. The scheme presented in general, and works with any quantum code, that satisfies certain restrictions, namely that it is a "proper quantum code". The constant threshold η_0 is a function of the parameters of the specific proper code used.

We present two explicit classes of proper quantum codes. The first class generalizes classical seret sharing with polynomials. The codes are defined over a field with p elements, which means that the elementary quantum particle is not a qubit but a "qupit". The second class uses a known class of quantum codes and converts it to a proper code.

We estimate the threshold η_0 to be $\simeq 10^{-6}$. Hopefully, this paper motivates a search for proper quantum codes with higher thresholds, at which point quantum computation becomes practical.

Genetics is Not in the Genes

Henri Atlan
Human Biological Research Center
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Abstract

The widely accepted metaphor of the genetic program is based on (i) a confusion between coding and programming, (ii) the fallacious assimilation of any binary (or quaternary) string to a computer program. Contrary to proteins and RNA, DNA by themselves are inert molecules, capable only to store information in their static structure, but not to trigger any genetic *activity* in the classical sense of what produces genesis and development.

An alternative metaphor was proposed where DNA strings are compared with data processed by the biochemical network of the metabolic cellular machinery working like a distributed program, rather than a program executed by this machinery. Respective advantages and disadvantages of the two metaphors are discussed. Instances of epigenetic inheritance argue in favor of the second metaphor, as well as processes of embryonic developments where the activity patterns of the DNA are determined by cytoplasmic events of maternal origins, themselves triggered and activated in the absence of the maternal genome.

It is concluded that a most adequate metaphor should be that of an evolving network where DNA and the metabolic network would work both as program and data at different time scales. Thus, what may be compared to the activity of a developmental program, being not located exclusively in the DNA, should be viewed as a dynamic system distributed on both the genome and the cellular machinery.

Speed vs. Quality in Low Bit-Rate Still Image Compression using Wavelets

Amir Averbuch[1] and *Moshe Israeli*[2]

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[2] Faculty of Computer Science, Technion, Haifa, Israel

Abstract

This paper presents a fast and modified version of the Embedded Zero-Tree Wavelet (EZW) coding algorithm that is based on [2,3,4] for low bit-rate still image compression applications. The paper presents the trade-off between the image compression algorithm speed and the reconstructed image quality measured in terms of PSNR. The measurements show a performance speedup by a factor of 6 in average over the EZW [4] and the algorithm presented in [3]. This speedup causes a PSNR degradation of the reconstructed image by 0.8–1.5dB in average. Nevertheless, the reconstructed image looks "fine" with no particular visible artifacts even if we have an average degradation of 1dB in PSNR.

The fast algorithm with its achieved speedup is based on consecutive application of four different techniques: 1. Geometric multi-resolution wavelet decomposition [5]. It contributes a speedup factor of 4 in comparison to the symmetric wavelet decomposition in [3,4]. It has a prefect reconstruction property which does not degrade the quality. 2. Modified and reduced version of the EZW algorithm for zero-tree coefficient classification. It contributes a speedup factor of 6 in comparison to the tree processing in [3,4]. It degrades the quality of the reconstructed image. 3. Multi-resolution data representation which enables fast and efficient traversing of the zero-tree. It does not degrade the quality, and 4. Exact model coding of the zero-tree coefficients. It contributes a speedup factor of 15 in comparison to the adaptive modeling in [3]. This is a loss-less step but reduces the compression rate. The paper presents a detailed description of the above algorithms accompanied by extensive performance analysis. It shows how each component contributes to the overall speedup.

The fast compression has an option of manual allocation of compression bits which enables a better reconstruction quality at a pre-selected "zoom" area.

The presented algorithm is inherently parallel, thus enabling implementation on commercially available off-the-shelf multiprocessor system architectures such as multi-DSP PC boards.

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Adaptive sparse solution of multidimensional elliptic problems

Amir Averbuch[1], *G. Beylkin*[2], *R. Coifman*[3], *P. Fischer*[4] and *M. Israeli*[5]

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Abstract

We consider efficient discretization and solution of PDEs which are forced by RHS with regions of smooth (non-oscillatory) behavior and possibly localized regions with non-smooth structures.

The efficient discrete representation of continuous operators is the basic problem in the numerical solution of differential and integral equations. Classical methods of discretization lead to dense representations for most operators. An important step in numerical computations consist of building sparse representations of common operators and algorithms for using them.

The method described in this paper is based on the wavelet transform which provides sparse representations of operator kernels. In addition the wavelet basis allows for automatic adaptation (using tresholding) in the sense that only a few coefficients are needed to describe smooth sections of the right hand side (r.h.s.) while more coefficients are needed for sharp transitions and for singular points. This economy is due to the vanishing moments property of high order wavelets.

In this work we develop adaptive algorithms, i.e. algorithms such that the number of operations performed is proportional to the number of significant coefficients in the wavelet expansion of the "inputs" of a given differential equation problem. We adapt an iterative approach thus we can succeed if we must do only a fixed number of iterations were each iteration requires a fixed number of operations, independent of the resolution (but dependent on the accuracy chosen).

The basic tool in our approach is the preconditioned conjugate gradient iteration in a "constrained" form. In the wavelet basis diagonal preconditioners are available which render the condition number of elliptic operators to O(1), This means that a constant number of iterations is required for solution to a prescribed accuracy. Each iteration consists of applying the non-standard-form of an operator to the wavelet expansion of a function, this translates to a multiplication

of a sparse vector by a sparse matrix. In the case of the non-standard-form the operator is a convolution and is represented by short filters, thus the number of operations is a constant multiple of the number of non vanishing elements in the vector. In addition we have sparse inner products and sparse multiplication by constants. The "constraint" is applied in a form of a mask such that only elements of the vector in the mask are used in the computation other elements are not generated. The implementation is performed using sparse data structures.

Multiscale Energy Minimizations for Simple Molecular Chains

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Abstract

Results for a multiscale algorithm for minimizing energy of bonded forces in 2D and 3D molecular chains are presented. The basic multiscale elements: relaxation, coarsening, interpolation and recursiveness are discussed. Bonded forces are divided into strong (local) and weak (long-range). In 2D these forces are bond lengths and angles respectively. In 3D the local forces are bond lengths and angles and the long-range force is the torsion. These entails a coarsening ratio of 1:2 in 2D and 2:5 in 3D. The fine grid relaxations are simple Gauss-Seidel point-by-point sweeps in 2D and relaxation on all triplets of adjacent atoms in 3D. Coarse to fine interpolations are derived from local sets of atoms. These sets include both fine and coarse atoms. All interactions between local set atoms and other atoms are ignored. Interpolation constants are derived by doing local relaxation sweeps on all fine-only atoms for several configurations of the coarse points in the set. In 2D the asymptotic convergence rates for realistic coupling strengths are ~ 0.1 for $V(1,1)$ cycles. Some intermediate results of a work in progress on 3D chains are presented as well.

Reduced Variable Molecular Dynamics: A Multi-Body Approach to Molecular Dynamics

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Abstract

Molecular dynamics is a major computational tool to study structure, dynamics and thermodynamics of molecules in general, and biomolecules in particular. Due to integration requirements conventional molecular dynamics (MD) simulations of large systems (e.g., proteins) is limited to short times on the order of nanoseconds. We have developed a new algorithmic approach to molecular dynamics which allow significant speedups while retraining a level of accuracy similar to that of standard MD. The approach makes use of the multi-scale hierarchy of protein structure and uses it to substructure the molecule to smaller (rigid or flexible) bodies connected by hinges. This separation, which involved several novel algorithmic developments, is combined with a multi-timestep to the integration. The results of the new program, denoted as CHARMM/MBO(N)D, give speedups of up to a factor of 20 while retaining good dynamic properties. The detailed example of the dynamics of the C-terminal domain of a ribosomal protein (1ctf) will be presented and discussed.

Bacterial Wisdom, Gödel's Theorem and Creative Genomic Webs

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Tel Aviv University
Tel Aviv, Israel

Abstract

The amazing process of evolution — from inanimate matter, through organisms of increasing complexity, to the emergence of intelligence — is claimed to be merely a successful accumulation of errors (random mutations) enhanced by natural selection (the Darwinian picture). The power of the Darwinian picture lies not only in its achievements, but also in the dismay evoked by what seems to be the only alternative — Vitalism.

But is Vitalism the only alternative? Or could there be another picture, neither Darwinian nor Vitalistic? This lecture is devoted to presenting an alternative approach. I propose a new evolutionary picture, where progress is not a result of successful accumulation of mistakes in replication of the genetic code, but is the outcome of designed creative processes.

I start with the classical experiments of Luria and Delbrück that demonstrated for the first time the existence of random mutations prior to the application of the selective pressure. A decade latter (during the 50's and early 60's) a number of major discoveries were made, of which only one (the double helix structure of the DNA) is widely known. I briefly review these important findings which should have changed the paradigm, since they showed that the genome is a dynamic entity capable of changing itself. These findings are a fundamental basis to our new picture of the genome. I continue with the recent developments in adaptive mutagenesis demonstrating direct mutation in response to a non-lethal selective pressure. In all of these experiments the selective pressure acts on the individual bacteria. My belief in cooperative genetic changes led me to a new experimental endeavor, in which the selective pressure was on the colony. The new experiments led to important new observations of morphotype transitions in stressed colonies. These are genetic changes which are beneficial to the colony but not directly to the individual cells. The observations led me to propose a new picture of the genome.

The genome, as I see it, is not merely a storage device, but a sophisticated cybernetic entity well beyond a universal Turing machine. Metaphorically speaking, it includes a user, a computational unit, and a hardware engineer and technicians. Namely, it is an adaptive cybernetic unit with self-awareness.

At first it seems that the assumption that the genome is an adaptive cybernetic unit with self-awareness will suffice to explain evolution. However, this is not so. A lemma extended from Gödel's theorem sets limitations on self-improvement. Naively phrased, it says that a system cannot design another system which is more complex than itself.

Based on the contemporary knowledge of genetic communication in a stressed colony, I propose that the colony forms a genomic web (I use the term web instead of network to emphasize that the building blocks are self-aware agents and not elements). The genomic web is a "super-mind" relative to the individual genome. The web is far more complex than the individual genome, so it can design a new and more advanced genome which would represent a vertical leap beyond the previous genomic version. It is best described as a cooperative self-improvement or cooperative evolution.

The fractal nature of randomly adsorbed objects

Ofer Biham, *Dani Lidar (Hamburger)*, *David Avnir*,
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Abstract

The fractal properties of randomly adsorbed objects on the plane are studied using the standard box counting and Minkowski techniques. It is found that even if the objects themselves are not fractals, and they are distributed with no correlations, for low coverage, fractal behavior is obtained for a range of scales between physically relevant cutoffs. The case of randomly distributed disks is solved analytically. It is shown that this model is an important limit of random fractal structures. It provides useful insight for common empirical systems of surface absorption, aggregation, laser ablation and porous media. In these systems the randomly distributed objects can be compact (disks), rod-like or fractals themselves. The model can also be considered as a first approximation for systems in which the distribution of adsorbed objects exhibits strong correlations.

For randomly distributed fractal objects we predict that there is a range of lengthscales in which the box counting function and the effective fractal dimension are determined by the distribution of objects rather than the object structure.

We also examine systems in which there is a power law distribution of distances (or object sizes), which gives rise to fractal structures. In this case an important issue is the origin of the power law distribution. The multiplicative dynamics with a lower cutoff, recently proposed by Solomon and Levy is examined in this context as a possible power-law-generating mechanism.

The Gauss Center Research in Multiscale Scientific Computation

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Abstract

The Carl F. Gauss Center for Scientific Computation was established in 1993 jointly by the Minerva Stiftung Gesellschaft für die Forschung m.b.H., Germany, and by the Weizmann Institute of Science, Rehovot, Israel. Its mission is the development of new fundamental computational approaches in physics, chemistry, applied mathematics and engineering, focusing in particular on advanced *multiscale* ("multi-resolution", "multilevel", "multigrid", etc.) methods.

Multiscale computation: general

It is well known that some of the major bottlenecks in science and engineering are computational in nature. The detailed understanding and design of large molecules, condensed matter and chemical processes, for example, could in principle be achieved just by computation, since the underlying equations are fully known; except that our computing capabilities are inadequate for such tasks. The same is true for the calculation of elementary particle properties from first principles, or for the design of fusion reactors or airplane maneuvers, and for many other engineering and scientific endeavors. All would be greatly facilitated if unlimited computing power were available — or if much better algorithms could be devised.

Indeed, just building ever faster machines will not do. With current computational methods the needed amount of computer processing often increases too steeply with the rise in problem size, so that no conceivable computer will be adequate. Completely new mathematical approaches are needed.

Most computational super-problems in science and engineering share some common features. For example, all of them involve a multitude of variables located in a low dimensional space (e.g., the four dimensional physical space-time). Closer examination reveals that the computational complexity of these problems results directly from this spatial nature, in several general ways that come up again and again, in different disciplines and in all kinds of guises. Past studies have demonstrated that such complexities can be effectively overcome, or drastically reduced, by multiscale algorithms.

Indeed, any many-variable problem defined in physical space can have an approximate description at any given length scale of that space: a continuum problem can be discretized at any given resolution; collective motions of a many-body system can be organized at any given characteristic length; etc. The multiscale algorithm recursively constructs a sequence of such descriptions at increasingly larger (coarser) scales, and combines local processing (relaxation of equations, simulation of statistical relations, etc.) at each scale with various inter-scale interactions. Typically, the evolving solution on each scale recursively dictates the *equations* (or the Hamiltonian) on coarser scales and modifies the *solution* (or configuration) on finer scales. In this way large-scale changes are effectively performed on coarse grids, based on information previously gathered from finer grids.

As a result of such multilevel interactions, the fine scales of the problem can be employed very sparingly, and sometimes only at special and/or representative small regions. Moreover, the inter-scale interactions can eliminate various kinds of difficulties, such as: slow convergence (in minimization processes, PDE solvers, etc.); critical slowing down (in statistical physics); ill-posedness (e.g., of inverse problems); large-scale attraction basin traps (in global optimization and statistical simulations); conflicts between small-scale and large-scale representations (e.g., in wave problems); numerousness of interactions (in many body problems or integral equations); the need to produce many fine-level solutions (e.g., in optimal control) or very many fine-level independent samples (in statistical physics); etc. Also, the multiscale interactions tend to bring out the large-scale dynamics, or the macroscopic equations, of the physical system, which is often the very objective of the entire calculation.

Since the local processing (relaxation, etc.) in each scale can be done in parallel at all parts of the domain (e.g., at all cells of a given lattice), the multiscale algorithms, based on such processing, are ideal for implementation on massively parallel computers. Indeed, many problems cannot be efficiently solved by such computers without employing a multiscale procedure.

Current research directions at the Gauss Center

Over the last three years, the research at the Gauss Center has involved the following directions.

1. New multigrid methods for steady-state fluid dynamics at all Mach and Reynolds numbers, and other non-elliptic stationary PDE systems.
2. Multilevel approaches to time-dependent partial-differential equations, emphasizing applications to oceanic and atmospheric flows.
3. Direct multigrid solvers for inverse problems, including system identification (e.g., impedance tomography) and data assimilation (in atmospheric simulations).

4. Optimal control: Feedback control via very fast updating of open-loop solutions, based on their multiscale representations.

5. Optimal location of singularities of PDE systems (e.g., location of the nucleons in electronic structure calculations), integrated into the multigrid PDE solver.

6. New multilevel algorithms for highly indefinite (e.g., standing wave) problems.

7. Multigrid solvers for the Dirac equations arising in quantum field theory.

8. Compact multiresolution representation of the inverse matrix of a discretized differential operator; fast updating of the inverse matrix and of the value of the determinant upon changing an arbitrary term in the matrix itself; with application to the QCD fermionic interaction.

9. Collective multiscale representation and fast calculation of many eigenfunctions of a differential operator, e.g., the Schrödinger operator in condensed-matter electronic-structures calculations.

10. Multiscale Monte-Carlo algorithms for eliminating both the critical slowing down and the volume factor in increasingly advanced models of statistical physics.

11. Multigrid Monte-Carlo approaches for solving the high-dimensional (several-particle) Schroedinger equation by real-time path integrals.

12. Introducing multiscale computations to many-particle calculations, including fast evaluation of forces, fast convergence to local and global ground states, fast equilibration, and large time steps, with application to molecular mechanics; a new approach to molecular dynamics, based on stochastic implicit time steps.

13. Multigrid methods for integro-differential equations, on adaptable grids, with applications to tribology.

14. Multiscale methods for the fast evaluation and inversion of the Radon transform; applications to X-ray tomography and airplane and satellite radar reconstruction.

15. Multiscale algorithms for early vision tasks such as surface reconstruction, edge and fiber detection, segmentation, and meaningful picture coarsening.

16. Rigorous quantitative theory for predicting the performance of multigrid solvers.

A survey of current developments, past publications and future perspectives in these various directions appears as the following report.

A. Brandt: The Gauss Center Research in Multiscale Scientific Computation, Gauss Center Report WI/GC–7.

Immune Cognition

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Abstract

The immune system is characterized by the ability to 1) specifically recognize the fine molecular structure of antigens, 2) remember and record its experiences, 3) learn to modify the kinetics, magnitude and phenotype of its responses to specific antigens, and 4) choose the appropriate response among various options. These attributes suggest that the immune system is a cognitive system (albeit, without consciousness). The emergence of cognition rests on 1) multiscale evolution at the levels of the species and the individual, and 2) on interactions between components that are degenerate, redundant, pleiotropic and dynamic. These components (molecules, cells) are fairly well known. Therefore, I recommend the immune system as a convenient subject for those interested in complex systems, cognition, emergence and the cure of disease.

Superparamagnetic Clustering of Data — The Definitive by Solution of an Ill-Posed Problem

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Abstract

Clustering is an important technique in exploratory data analysis, with applications in image processing, object classification, target recognition, data mining etc. The aim is to partition data according to natural classes present in it, assigning data points that are "more similar" to the same "cluster". We solved this ill-posed problem without making any assumptions about the structure of the data, by using a physical system as an *analog computer*. The physical system we use is a disordered (granular) magnet. The method was tested successfully on a variety of artificial and real-life problems, such as classification of flowers, processing of satellite images, speech recognition and identification of textures and images.

Coherent Structures Extraction and Computation in Two-Dimensional Turbulence Using Wavelets

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Abstract

Fully developed turbulence, namely the study of *highly nonlinear flows*, is a challenge for mathematicians and physicists. It remains an unsolved problem because our present conceptual and technical tools seem inadequate.

Turbulent flows are deterministic systems sensitive to initial conditions; therefore their behaviour can only be predicted statistically. Two possible statistical approaches have been tried: — either a *kinetic approach*, introduced by Reynolds in 1894, which considers time or space averages and separates flow fields into mean and fluctuating motions, supposing their temporal or spatial scales are sufficiently decoupled (spectral gap hypothesis), — or a *probabilistic approach*, introduced by Kolmogorov in 1941, which considers ensemble averages and describes flow fields as random functions characterized by their probability law. Both approaches are difficult to justify, because: — the kinetic approach relies on the *spectral gap hypothesis*, which is not valid, — the probabilistic approach predicts the behaviour of ensemble averages, but the relation of these to time averages measured in laboratory or numerical experiments depends on the validity of the *ergodic hypothesis*, which is not proven.

Our talk will be focused on two-dimensional turbulence, which is encountered in large-scale atmospheric and oceanic flows. The probabilistic approach has led to the *statistical theory of two-dimensional turbulence*; it predicts a direct entropy (integral of the squared vorticity) cascade with a power-law spectrum in k^{-3} and an inverse energy cascade with a power-law spectrum in $k^{-5/3}$. Such a spectral behaviour, presenting an accumulation of energy in the large scales, is characteristic of long-range dependence.

We will show that the predictions of the statistical theory are not verified in direct numerical simulations of two-dimensional turbulence, because the observed spectral slope is steeper than the predicted one. We conjecture that this discrepancy is due to the formation of *coherent structures*, namely isolated vortices embedded in a *background flow of vorticity filaments*, produced when the vortices strongly interact and are then randomly advected by them. We also con-

jecture that the coherent structures are responsible of the long-range dependence we observe.

To analyze this long-range dependence we have introduced wavelets and wavelet packets (self-similar wave packets) techniques to separate the coherent structures from the background flow [Farge and Rabreau, 1988], [Farge, 1992], [Farge *et al.*, 1992], [Farge *et al.*, 1996]. We have shown that the coherent structures correspond to the strong wavelet coefficients while the vorticity threads correspond to the weak wavelet coefficients, both components are multi-scale but present different scaling laws. This has led us to define *conditional averages*, we have used to prove that the coherent structures are responsible for the steepening of the spectral slope [Farge, 1994].

In computing separately the coherent structures and the background flow evolutions, we have also shown that the coherent structures inhibit the nonlinear instabilities in their vicinity [Kevlahan and Farge, 1996], which gives us some evidence of a *wavelet gap*. We use this gap to define a new method to model two-dimensional turbulent flows. It is based on the computation of Navier-Stokes equations in a wavelet basis, compressed at each time step to discard the weakest wavelet coefficients, which models the entropy dissipation. In order to obtain a statistically stationary regime we force the flow in exciting the strongest wavelet coefficients (corresponding to the coherent structures), which models the local production of vortices in shear or boundary layers [Farge and Schneider, 1996].

In conclusion we have some justification for attempting to construct a *kinetic theory of two-dimensional turbulence* based on coherent structures. The vorticity field is represented as a superposition of vortices having a deterministic behaviour with long-range interactions, embedded in a random background flow which is modelled by a Gaussian stochastic forcing, whose amplitude depends on the probability of vortex strong interactions.

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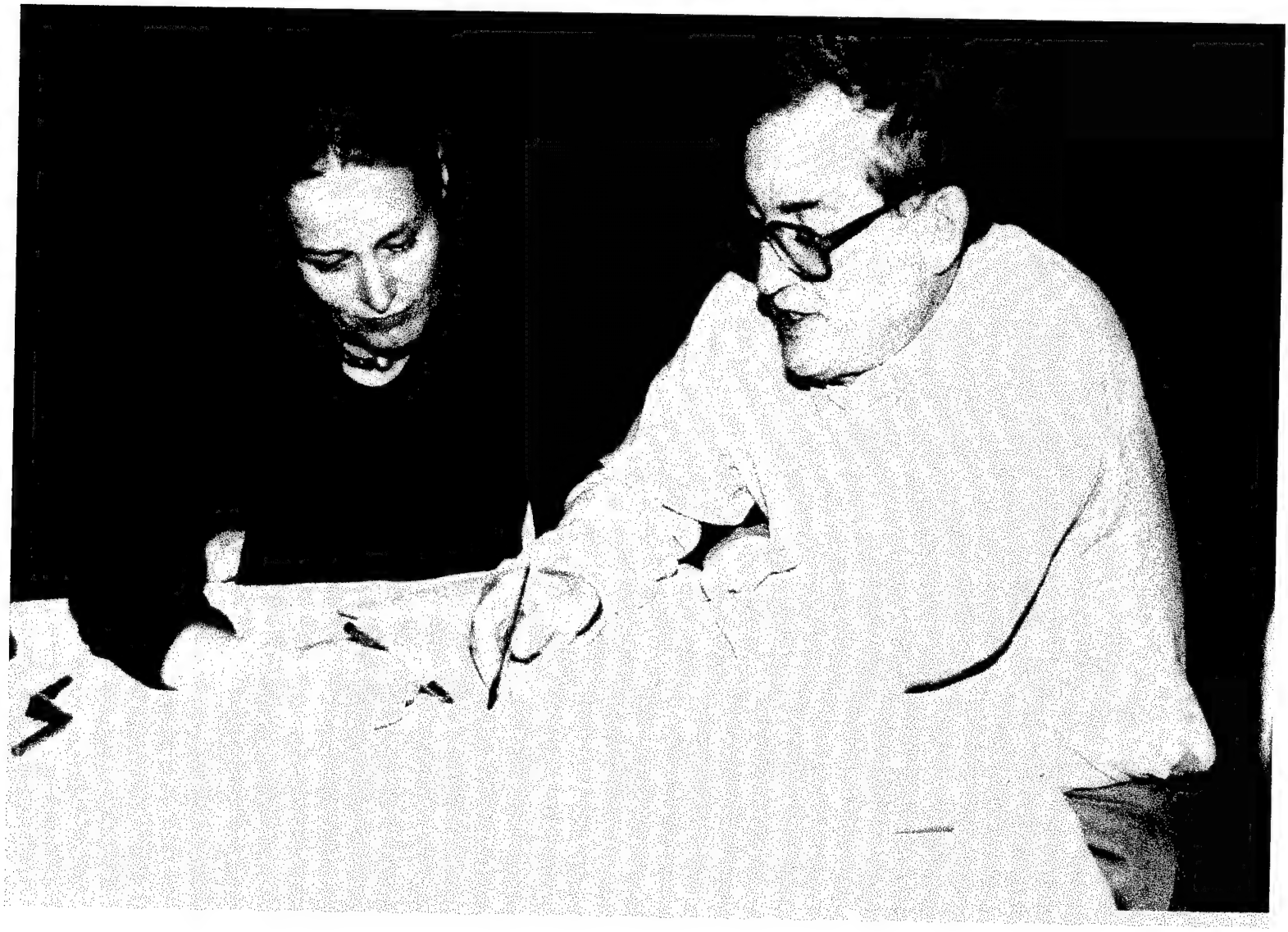

Gerhard Mack and Marie Farge comparing a red marker with a blue ball point pen

Numerical Study of the Schrödinger Equation in a Wavelet Basis

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Abstract

The BCR (Beylkin-Coifman-Rokhlin) algorithm is used to represent matrices in a particular sparse form called the "Non Standard" form.

The operator corresponding to the Schrödinger equation is decomposed on an orthonormal wavelet basis for the simple case of hydrogenlike atoms.

Using this particular representation, the Lanczos method is used to solve the eigenvalue problem related to this operator.

Physical quantities as energies are numerically computed and compared with their theoretical values to test the validity of the process. The process is also used to compute the 5^{th} excited state of a pseudo-double well potential.

Software Development Center. Conception of "Black Hole"

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Abstract

The first lepton has changed our world

In accordance with the Standard Model, Matter consists of quarks and leptons. The first lepton — electron with a mass of 0.5 Mev was discovered at the very end of XIX Century. It became the basis for XX Century technology.

We have yet to see what the remaining two leptons, μ and τ will offer our civilization, but for the present time, we have still a great deal to learn and work with in our current level of electronic technology.

Prodence Software Ldt.

Prudence Software Ltd. established in 1997 is a new Software Development Center located in Jerusalem. The Center was started with cooperation of the U.S. company Elmasoft, Inc. acting as a strategic partner. The Center has already made good professional contacts with Accelerator Laboratories in U.S.A., Europe and Japan.

Electromagnetic software

Prudence Software is developing electromagnetic codes (computational programs) for the solution of electromagnetic and electrodynamics problems for industry and scientific research. The applications of EM codes are wide ranging from precise electronic devices to power components of Particle Accelerators (the main instruments of Fundamental Physics and High Energy Physics.)

Integrated complex

A new generation of EM codes to meet the modern needs and requirements of physicists, engineers and designers will be developed. All codes will be united in the Integrated Complex providing beam dynamics simulations and the design of a set of EM components, such as the following:

* Electron and ion sources;
* RF (radio frequencies) systems;
* Magnet systems and others.

The codes will be able to interact with each other due to their inherent properties:

* Identical structure of data;
* Identical organization of pre- and post-processors;
* Identical Graphic User Interface;
* Prompt transfer to different platforms.

Product line

* "Off the shelf" codes;
* "Tailor made" codes;
* "Rough but Quick" codes (RBQ-codes);
* The last option gives the possibility for the user to communicate with the program through professional language only.

Numerical methods

* Finite Elements Method;
* Boundary Elements Method;
* Finite Differences Time Domains;
* Multigrid Methods.

What is EM software for?

It is an essential tool for every electronics developer, as basic as an oscillograph. But unlike the oscillograph, EM Software is used from the very first stages of design where there exists only physics idea, and later — for the construction, testing and manufacturing EM codes significantly reduce time of design and the risk attached to innovation.

Structure of the center

* Development Laboratory;
* Software Factory;
* Advanced Group for permanent contacts with customers and partners;
* Business Management.

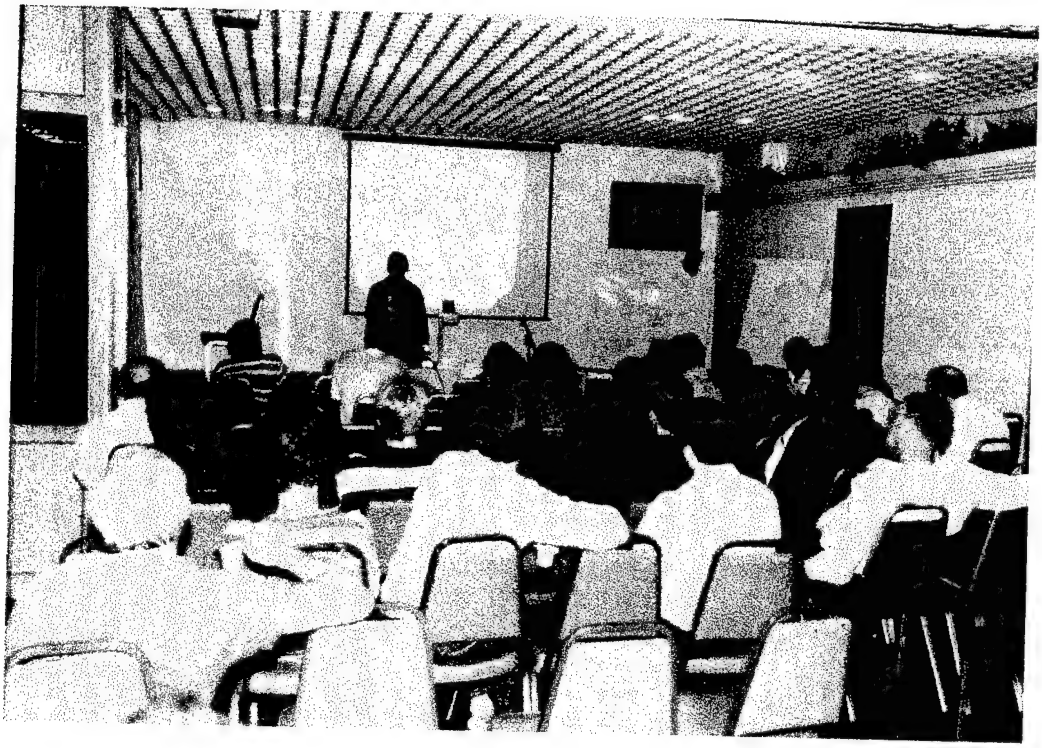
2/3 of the Center development staff are Ph.D.s in Physics and Mathematics.

Prudence club

A professional and intellectual environment associated with the Center created to the interact with the staff. A list of the Club members currently includes 15 firstclass experts in physics, mathematics, programming and engineering.

Conception of "Black hole"

In comparison with the rapid changes in experimental physics and in the high-tech industry, the develoment of new computational codes is not keeping pace. The activities of many small teams is uncoordinated as it is should be for such a multidisciplinary product. Conception of "Black Hole" means an intention of the Development Center plans to be strongly attractive for those who have a "mass" of ideas, experience and issues in computational physics, mathematics and engineering.



Boris Fomel at the screen in the main lecture hall

Universal Formulae for Percolation Thresholds

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Abstract

A power law is postulated for both site and bond percolation thresholds. The formula writes $p_c = p_0\left[(d-1)(q-1)\right]^{-a} d^b$, where d is the space dimension and q the coordination number. All thresholds up to $d \to \infty$ are found to belong to only three universality classes. For first two classes $b = 0$ for site dilution while $b = a$ for bond dilution. The last one associated to high dimensions is characterized by $b = 2a - 1$ for both sites and bonds. Classes are defined by a set of value for $\{p_0;\ a\}$. Deviations from available numerical estimates at $d \leq 7$ are within ± 0.008 and ± 0.0004 for high dimensional hypercubic expansions at $d \geq 8$.

The formula is found to also yield Ising critical temperatures.

Do Humans Behave Like Atoms

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Abstract

Competing bimodal coalitions among a group of actors are discussed. First, a model from political sciences is revisited. Most of the model statements are found not to be contained in the model. Second, a new coalition model is built. It accounts for local versus global alignment with respect to the joining of a coalition. The existence of two competing world coalitions is found to yield one unique stable distribution of actors.

On the opposite a unique world leadership allows the emergence of unstable relationships. In parallel to regular actors which have a clear coalition choice, "neutral", "frustrated" and "risky" actors are produced. The cold war organization after world war II is shown to be rather stable. The emergence of a fragmentation process from eastern group disappearance is explained as well as continuing western stability.

Some hints are obtained about possible policies to stabilize world nation relationships. European construction is analyzed with respect to European stability. Chinese stability is also discussed.

Optimal Multigrid Calculations of Thermodynamic Limits

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Abstract

We present a class of multigrid Monte Carlo algorithms that calculate thermodynamic limits very efficiently. In addition to the elimination of the "critical slowing down", the "volume factor" can be also eliminated. That is, the need to produce many independent fine-grid configurations for averaging out their statistical deviations is removed, by applying multigrid cycles that sample mostly on coarse grids. Thermodynamic limits can be calculated to relative accuracy ε_r in optimal time which is just $O(\varepsilon_r^{-2})$ computer operations, where ε_r is the error relative to the standard deviation of the observable. Note that in the usual Monte Carlo process one would need $O(N^{d+2}\varepsilon_r^{-2})$ computer operations in order to obtain a relative error of order ε_r, for a d-dimensional lattice with linear dimension N. We will present our optimal multigrid methods and the numerical results for the Gaussian models, including the massive Gaussian model and the variable-coupling Gaussian model. Our recent study of the anharmonic crystal model will be discussed.

Is the Fast Multipole Method Fast?

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Abstract

Since its formulation by Greengard and Rokhlin [1] a decade ago, the fast multipole method (FMM) has been regarded as one of the most promising approaches to the fast summation of electrostatic interactions in systems containing large numbers of charges. In contrast to primitive summation methods, which have an asymptotic computational complexity of $O(N^2)$ (where N is the number of charges), the FMM achieves $O(N)$ complexity by utilizing multipole expansions for the calculation of interactions between well-separated groups of charges within the framework of a hierarchical tree structure. Obviously, use of the FMM becomes advantageous (at least relative to primitive methods) for sufficiently large N (i.e. for N larger than some "breakeven" value N_c). The main practical question is, how large is N_c, and, consequently, for which envisioned applications is the FMM likely to useful? For periodic systems, this question is further complicated by the existence of other fast summation methods including the optimized Ewald method (with $O(N^{3/2})$ complexity) and FFT-based methods such as the particle-particle particle-mesh (P^3M) and particle-mesh Ewald (PME) (both with $O(N \log N)$ complexity). A number of studies of the FMM method have been carried out in recent years, but estimates of its efficiency relative to competing methods vary wildly, and no concensus as to its usefulness has emerged.

We give a brief introduction to the FMM, discuss some of the improvements to the method that have been proposed, and then survey some recent studies of the performance of the FMM in an attempt to make sense of the situation, with a focus on fast summation of long-range interactions in the context of molecular simulation. Our overall conclusion is that more systematic comparative studies of algorithms for the fast summation of long-range interactions are badly needed, and that a forum for the effective testing and evaluation of competing methods should be created.

Reference

[1] Greengard, L. and V. Rokhlin, *J. Comput. Phys.* **73** (1987) 325.

Algorithms for New Products Development [An Exercise in Thought Dynamics]

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Abstract

We generate new product ideas using algorithms which manipulate formally conceptual structures. These structures are abstract closed configurations composed of discrete elements which represent parts or properties of the products and of their immediate environment. The algorithms are assembled of a very limited number of fundamental operations acting on the elements. We present some successful field applications of the method carried out in leading international companies as well as an experiment providing quantitative proof of its superiority over usual ideas search.

1. Introduction

Inventing new things is considered as the ultimate intrinsically human activity. It is usually considered to be a highly complex process and as such, difficult to formalize and control.

The present work is an extension of our former study [1] of creative thought in advertising. We chose this as our initial application because it is a rather closed conceptual system (independent on external factors such as physical laws, engineering parameters, etc.). In the process of extending our methods to other creative activities, we address in the present paper the automatic creation of new products. New Products Development (NPD from now) turns out to be representable too as a closed system whose intrinsic dynamics can be characterized by rather simple and well defined elementary interactions. Such systems admit a rather systematic treatment by methods extending the traditional methods of Statistical Mechanics [2,3].

In particular, in spite of a limited set of fundamental rules, the phase space of the system has a large dimensionality. One of the typical phenomena for such systems is critical slowing down: the exploration of the system properties (ground states, susceptibility to external parameters etc.) takes a divergently large time. In the context of manipulating creative concepts, this translates in very long times for producing really innovative and successful ideas.

The usual solution in the context of Statistical Mechanics is the identification of effective collective degrees of freedom and devising algorithms which act directly in terms of theses macroscopic degrees of freedom (macros [4]). Such procedures replace the slow dynamics based on random walk by a dynamics relying on macroscopic steps. The macroscopic steps are devised such as to express the motion of the system along the relevant directions in the phase space. The present work proposes to extend these techniques to the process of inventing new products. We have chosen new marketable products (rather than creative art or poetry for instance) because of the quantitative tools available for validating results (see section 5 for the experimental validation of our algorithms).

The existing methods for searching new product ideas (brain storming, random stimulation etc. [5]) are similar to random walks. We suggest, by analogy to Statistical Mechanics, to substitute this random walk dynamics by the analog of cluster-multiscale algorithms. By including in the stochastic dynamics knowledge on the relevant global moves (macros) one hopes to accelerate very significantly the dynamics of the system and improve its efficiency. Thus we would reproduce in the NPD context the capability of the cluster-multiscale algorithms to transcend Critical Slowing Down [4].

In order to apply such techniques, one has to ascertain that the system is to a good approximation isolated from external changes and that its global dynamics can be expressed in terms of discrete degrees of freedom. These requirements might seem problematic in the context of marketable products:

- according to the common lore. NPD is driven by changes in the (external) market forces and technology.
- creative thinking is usually considered to be a fluid, unstructured process.

However, in the case of generating creative advertisement ideas, it has been shown [1] that thinking could be treated as a closed system of discrete elements and operations. The importance of a finite system was also emphasized for inventive problem solving in engineering [6]. The decisive proof that this approach extends to NPD is provided by the phenomenological success (section 7) of the algorithms based on our discrete representation.

The relevant degrees of freedom and the operations are assembled in a set of algorithms which were isolated initially from experimental data. Indeed, theses conceptual structures reoccur systematically in the natural dynamics of successful NPD in the same way in which relevant collective structures (like instantons, solitons, vortices) appear in the natural statistical mechanics of various physical systems. The systematic restructuring of the natural inventive thinking was pioneered in the context of engineering problem solving by Altschuler [7].

The main practical steps implementing our theoretical approach are: – Large sets of highly creative ideas sharing the same structure are identified and clas-

sified into classes.

- For each class, we define a standard "mechanical" algorithm which, when applied to an existing product, generates a new product idea belonging to the class.

The structure of the paper is as follows: In the next section we explain why, as opposed to the current view in the marketing community, the NPD process can be treated for most practical purposed as a closed system.

In section 3 we define the elementary degrees of freedom and their fundamental interactions.

In sections 4 and 5 we describe a few algorithms and illustrate their global dynamics on real-world examples.

In section 6 we present case studies of our method which were successfully completed by experts belonging to international leading companies (Ford, Motorola, etc.).

In section 7 we prove quantitatively that applying the dynamics of section 5 leads to results superior to the usual NPD procedures.

In section 8 we offer our conclusions and outlook.

Cluster Concept Dynamics Leading to Creative Ideas Without Critical Slowing Down

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Abstract

We present algorithmic procedures for generating systematically ideas and solutions to problems which are perceived as creative.

Our method consists of identifying and characterizing the most creative ideas among a vast pool. We show that they fall within a few large classes (archetypes) which share the same conceptual structure (Macros). We prescribe well defined abstract algorithms which can act deterministically on arbitrary given objects. Each algorithm generates ideas with the same conceptual structure characteristic to one of the Macros. The resulting new ideas turn out to be perceived as highly creative.

We support our claims by experiments in which senior advertisement professionals graded advertisement ideas produced by our method according to their creativity. The marks (grade 4.6=0.2 on a 1–7 scale) obtained by laymen applying our algorithms (after being instructed for only two hours) were significantly better than the marks obtained by advertising professionals using standard methods (grade 3.6=10.2).

The method, which is currently taught in USA, Europe and Israel and used by advertising agencies in Britain and Israel has received formal international recognition.

M.C. Simulations of Biomolecule-Water Systems

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Abstract

Water can be considered the most abundant and essential bio-molecule: no life as we know it can exist without water. All other bio-molecules (proteins, DNA, etc.) have evolved in water and need water to find their functional conformations and to perform their biological functions. Hence we have to consider water if we want to simulate bio-molecular systems. Water molecules are highly mobile and for relevant simulations it is necessary to include many water molecules. Hence, the presence of explicitly modelled water molecules in Molecular Dynamics or Monte Carlo simulations leads to two restrictions: 1. it allows only for small time steps or moves, and 2. it makes each time step or move expensive in terms of CPU-time. Today, these restrictions mean that the time scale accessible via simulations extends to nanoseconds. However, many processes of biological relevance occur on much longer time scales. If one is not aiming at the simulation of short term events, water can be treated as a continuum. Then the most important energetic contribution of water, namely electrostatics, can be calculated by solving the Poisson-Boltzmann equation (see e.g. B. Honig and A. Nicholls, *Science* **268** (1995) 1144–1149). We (in collaboration with Takumi Washio, NEC, and Kees Oosterlee, GMD-SCAI, both in St. Augustin, Germany) propose to combine fast multigrid methods for the solution of the Poisson-Boltzmann equation with an efficient Monte Carlo scheme for bio-polymers (see D. Hoffmann and E.W. Knapp, *Eur. Biophys. J.* **24** (1996) 387–403). Alternative ways of treating water are also discussed, e.g. larger moves using explicitly modelled water molecules.

Combining Multicanonical Reweighting with Multigrid and Cluster Algorithms

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Abstract

Canonical Monte Carlo simulations of first-order phase transitions are severely hampered by the occurrence of very rare states containing interfaces which are extremely important to achieve equilibrium in finite-size systems. Compared to configurations of the pure phases they are exponentially suppressed by a factor $\exp(2\sigma L^{d-1})$, where σ is the (reduced) interface tension, L is the linear size of the system, and d is the dimension. This in turn leads to exponentially diverging autocorrelation times and hence to exponentially large statistical errors. A similar behaviour is observed in many disordered systems.

A way to overcome this problem is the multicanonical reweighting method. By updating the fields or spins with a local Metropolis or heat-bath update algorithm, the size dependence of the autocorrelation times can be reduced to a power law, $\tau \propto V^{\alpha}$, with α typically around 1.3. After a brief review of the basic idea, combinations of multicanonical reweighting with *non-local* update techniques will be discussed.

It is first shown that a combination with the multigrid algorithm further improves the performance of the simulations by roughly one order of magnitude, uniformly for all system sizes. Special emphasis will then be placed on the recently proposed "multibondic" algorithm which combines the reweighting idea with cluster updates. In this way the exponent α in the power law can be reduced to unity, the optimal value one would expect from a random walk argument. Asymptotically for large system sizes the new algorithm therefore always performs better than the standard multicanonical method.

Hierarchical Thinking in Developmental Biology

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Abstract

Today it is known that development is a hierarchical process, with successive decisions by cells to follow ever more refined pathways. Here, I describe work related to the progressive definition of cell fate and organ formation in the central nervous system.

Cells of the dorsal Vertebrate ectoderm become, under the induction of the Spemann organizer, the precursors of the neural plate. Cells in this plate in turn will give rise to neurons, glia and a variety of other cell types. This happens due to further events in the genetic cascade; in particular, certain of the genes involved form a cell-cell communication system of ligands (membrane molecules) and receptors (other membrane molecules "designed" to sense the presence of ligands on neighboring cells). While this process of determination is taking place, the neural plate invaginates to form a *tube*. The molecular hierarchy of genes responsible for cell determination and cell movement is becoming unravelled.

A computer model was built in order to better understand neural tube formation. This model correctly accounts for the phenomena just described. However, changes in certain parameters, in particular those related to cell-cell communication, lead to very different morphologies and cell-type distributions. It turns out that these unexpected configurations are appropriate to central nervous system formation in Invertebrates. Vertebrates and Invertebrates have very different central nervous systems; yet it has become fairly clear that the genes involved in both cases are the same. The computer model reconciles these two facts in a biologically plausible way, and leads to a proposal for the mechanism by which the evolutionary branching of the two Orders took place.

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Dynamical Explanation for the Emergence of Power Law in a Stock Market Model

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Abstract

Power laws are found in a wide range of different systems: From sand piles to word occurrence frequencies and to the size distribution cities. The natural emergence of these power laws in so many different systems, which has been called self-organized criticality, seems rather mysterious and awaits a rigorous explanation. In this letter we study the stationary regime of a previously introduced dynamical microscopic model of the stock market. We find that the wealth distribution among investors spontaneously converges to a power law. We are able to explain this by simple general considerations. We suggest that similar considerations may explain self-organized criticality in many other systems. They also explain the Levy distribution.

Power Laws are Logarithmic Boltzmann Laws

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Abstract

Multiplicative random processes in (not necessarily equilibrium or steady state) stochastic systems with many degrees of freedom lead to Boltzmann distributions when the dynamics is expressed in terms of the logarithm of the elementary variables. In terms of the original variables this gives a power-law distribution. This mechanism implies certain relations between the constraints of the system, the power of the distribution and the dispersion law of the fluctuations. These predictions are validated by Monte Carlo simulations and experimental data. We speculate that stochastic multiplicative dynamics might be the natural origin for the emergence of criticality and scale hierarchies without fine-tuning.

Spontaneous Scaling Emergence in Generic Stochastic Systems

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Abstract

We extend a generic class of systems which have previously been shown to spontaneously develop scaling (power law) distributions of their elementary degrees of freedom.

While the previous systems were linear and exploded exponentially for certain parameter ranges, the new systems nonlinear time evolution equations similar to the ones encountered in Spontaneous Symmetry Breaking (SSB) dynamics and evolve spontaneously towards "fixed trajectories" indexed by the average value of their degrees of freedom (which corresponds to the SSB order parameter). The "fixed trajectories" dynamics evolves on the edge between explosion and collapse/extinction.

The systems present power laws with exponents which in a wide range ($\alpha < -2$) are universally determined by the ratio between the minimal and the average values of the degrees of freedom. The time fluctuations are governed by Levy distributions of corresponding power. For exponents $\alpha > -2$ there is no "thermodynamic limit" and the fluctuations are dominated by a few, largest degrees of freedom which leads to macroscopic fluctuations, chaos, and bursts/x.

Simulating Ising Spin Systems on a Quantum Computer

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Abstract

A polynomial-time algorithm is presented for the construction of the Gibbs distribution of configurations in the Ising model, on a quantum computer. The algorithm is designed so that each run provides one configuration with a quantum probability equal to the corresponding thermodynamic weight. The partition function is thus approximated in the most efficient way. The algorithm neither suffers from critical slowing down, nor gets stuck in local minima, unlike most Monte Carlo simulations of spin glasses. It performs polynomially better than classical algorithms in finding the ground state of a class of spin glasses. The algorithm can be applied in any dimension, to short-range spin-glass Ising models with a finite portion of frustrated plaquettes, diluted Ising models, and models with a magnetic field.

Multigrid Methods for Standing Wave Equations

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Abstract

In this work we present a new multigrid solver for the standing wave equations with radiation boundary conditions.

The straightforward application of standard multigrid technique cannot provide an efficient solver to these equations, since some special Fourier error components (with frequencies depending on the wave number) have no efficient reduction: They are almost invisible for any relaxation on the fine grids and have no accurate approximation on the coarse grids. Therefore, this type of error needs special treatment. Our approach is based on the fact that each such problematic error can be factorized by representing it as the product of a certain high-frequency Fourier component and a smooth envelope function. The idea is then to reduce this type of error by approximating these smooth envelope functions on the coarse grids. An additional advantage of this approach is that it allows a natural introduction of the radiation boundary conditions.

*Introduction to the Renormalization Group**

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Abstract

I discuss the real space renormalization group (RG). Its purpose is to study systems with *random fluctuations* and *nonlinearities* which show *emergent behaviour*, i.e. nonlocal phenomena emerge from local interactions.

Examples include lattice models of statistical mechanics and of Euklidean quantum field theory which show correlations over large distances compared to the lattice spacing.

Given a more fundamental theory, the RG furnishes an *effective theory* which determines the outcome of all "macroscopic" measurements with spatial resolution $\Delta x = l$. The effective theory has much fewer degrees of freedom than the original theory. For instance it could live on a "block" lattice of lattice spacing l, with sites x, random variables $\Phi(x) \equiv \Phi_x$ attached to sites x, and a probability distribution

$$dprob(\Phi) = Z^{-1} \exp\left(-\mathcal{H}_{eff}(\Phi)\right) \prod d\Phi_x.$$

Mathematically, $dprob(\Phi)$ is a conditional expectation value of the probability distribution of the random variables of the original system.

Well known examples of effective theories include electrodynamics of polarizable media, equilibrium and nonequilibrium statistical mechanics.

What are the macroscopic variables $\Phi(x)$ and what does $\mathcal{H}_{eff}$ look like?

past state of the art: variables $\Phi(x)$ are some spatial averages of the same type as the fundamental variables $\varphi(z)$, and the effective Hamiltonian $\mathcal{H}_{eff}$ looks like the fundamental Hamiltonian $\mathcal{H}$, except for some changes in parameters. These changes are called *renormalization.*

future state of the art: Allow for the emergence of new degrees of freedom ("macros"): collective modes, composite objects, (local) topological charges (like vorticity) etc. They are determined from the requirement that $\mathcal{H}_{eff}$ *stays local.* $\mathcal{H}_{eff}$ may be very different from $\mathcal{H}$.

* Work supported in part by German Israel Foundation.

For instance, in a superconductor, composite scalar fields which describe Cooper pairs will appear in effective theories when the cutoff l^{-1} is low enough.

How does one compute $\mathcal{H}_{eff}$? Suppose the macroscopic variables $\Phi(x)$ have been defined as functions of the original variables (This is called "choice of block spin"), $\Phi(x) = C\varphi(x)$, where C is a linear or nonlinear restriction map. Then

$$\exp\left(-\mathcal{H}_{eff}(\Phi)\right) = \int \prod_x \delta\left(C\varphi(x) - \Phi(x)\right) \exp\left(-\mathcal{H}(\varphi)\right) \prod_z d\phi_z$$

in a lattice model. The δ-function may be regarded as a limit of a Gaussian. One increases the length scale l in several steps if necessary. If the scale factor l_{i+1}/l_i is small enough, the integral can be evaluated approximately by a saddle point approximation. As a lowest approximation to $\mathcal{H}_{eff}$ one obtains the minimum $\mathcal{H}_{perf}(\Phi) = \mathcal{H}(\Psi[\Phi])$ of $\mathcal{H}(\varphi)$ subject to the constraint that $C\varphi = \Phi$. It is assumed at $\varphi = \Psi[\Phi]$. The quantity $\mathcal{H}_{perf}$ is called the classical perfect action. The next correction involves $tr\ \ln \mathcal{H}''$, the logarithmic trace of the Hessian.

How does one detect the necessity to include extra variables $\Phi(x)$*?* In principle from the fact that $\mathcal{H}_{eff}$ becomes nonlocal otherwise. In a saddle point approximation, the nonlocality arises from low lying eigen-modes of the Hessian $\mathcal{H}''(\varphi = \Psi[\Phi])$. The Hessian is a matrix $\mathcal{H}'' = (\mathcal{H}_{,zw})$

$$\mathcal{H}_{,zw} = \frac{\delta^2}{\delta\varphi(z)\delta\varphi(w)}\mathcal{H}(\varphi = \Psi[\Phi]).$$

Its inverse $(\mathcal{H}'')^{-1}$ must decay with distance $|z - w|$ with decay $< l$. Otherwise the lowest eigenmodes have to be used to construct the extra variables Φ. This is discussed in detail in M. Grabowski's thesis. For this and other references see

http://lienhard.desy.de/ ~mackag/publications.html

Computational Fluid Dynamics of Geophysical and Astrophysical Phenomena

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Abstract

The fluid dynamics of the Earth's ocean and atmosphere, planetary and stellar atmospheres, and interplanetary ionized and neutral gases are a scientifically important and technically challenging subject for computational physics. The phenomena in these media are inherently multi-scale because of their turbulence, and the size of relevant computations is correspondingly large. Two specific examples are discussed: (1) the behavior of coherent magnetic vortices and current sheets in 3D, anisotropic magnetohydrodynamics, and (2) natural variability and abrupt transitions in the Earth's climate associated with the thermohaline circulation in the ocean.

Dirac Operator Spectrum and Random Matrix Models

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Abstract

Ensembles of complete spectra of the lattice Dirac operator for staggered fermions are calculated for SU(2) gauge fields. The accumulation of eigenvalues near zero is analyzed and compared with the predictions of the chiral random matrix model. A remarkable agreement for the distribution of the smallest eigenvalue and the microscopic spectral density is found.

Fast Multigrid Solvers for Higher Order Upwind Discretizations of Convection-Dominated Problems

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Abstract

In this talk we present new multigrid line smoothers for solving higher order discretizations of scalar convection-dominated problems directly. The behavior of the smoothers is analyzed with Fourier smoothing analysis. A parallel tri-line variant is presented and evaluated. The smoothers are applied to convection-diffusion problems, discretized with a limiter and systems of Navier-Stokes and Euler equations.

1. Introduction

The multigrid treatment of higher order finite difference or finite volume discretizations of convection-dominated problems, on the basis of van Leer's κ-schemes, is usually not as efficient as for Poisson-like problems. These discretizations are often solved indirectly with a defect-correction technique, where multigrid is used for solving the first order discretization. The higher order discretization scheme is then used as an outer iteration. In the defect-correction approach often the outer iteration determines the convergence speed, which can be slow if the first and higher order discretizations are very different.

A second popular approach in which higher order discretizations are solved directly in multigrid is with help of multistage smoothers. These smoothers are point smoothers of Jacobi-type and are therefore limited in their robustness with respect to problems discretized on grids with stretched cells.

In this talk a robust alternative to the two approaches mentioned above is presented, in which the higher order upwind discretization is also solved directly in multigrid. We present line smoothers based on a splitting of the operator into a 'positive' part in the left-hand side and a remaining (higher order minus positive) part. The smoothers based on this splitting can be of alternating, symmetric or zebra type and are called KAPPA smoothers here. The resulting splitting is analyzed with Fourier smoothing analysis for a linear convection diffusion equation discretized with the κ-scheme, similar to Wesseling (for the standard upwind discretization). A parallel variant is a tri-line zebra smoother, due to the fact that

a higher order 1D upwind stencil contains 4 elements. It is evaluated, whether the parallel smoother is an interesting competitor for the robust (non parallel) symmetric alternating line smoother. The theoretical results are compared to the actual multigrid convergence for model problems. In two-grid Fourier analysis we observe the discrepancy between the scaling of convection and diffusion on fine and coarse grids. For the 'inflow/outflow' problems evaluated here we will not see the negative effect of the different scaling on the multigrid convergence, due to the influence of the combination of Dirichlet boundary conditions and the line smoothers, which reduce not only high-frequency, but also low-frequency error components.

The multigrid solution method used here is the nonlinear FAS scheme, because we will also investigate the influence on the multigrid convergence of discretization schemes with a limiter. Numerical tests for convection-dominated scalar problems are performed on fine grids. Furthermore, the smoothers are tested for an incompressible Navier-Stokes and a compressible Euler example.

A Little Study on Analyticity Properties of the Ising Renormalization Group

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Abstract

Analyticity properties of the first (block spin) renormalization group step for the 2D Ising model are studied by exact calculations on small lattices. By computing the zeroes of the effective Boltzmannians in the complex $\exp(4\beta)$ plane, evidence is provided that the effective Hamiltonians are free from singularities in the neighborhood of $\beta = \beta_c$.

Preconditioning in Conjugate Gradient-like Methods by Symmetric Multigrid Algorithms

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Abstract

Usually the algebraic system obtained after a (classical) finite element discretization of an elliptic (nonsymmetric) boundary value problem is ill-conditioned. Thus,most of the conjugate gradient (CG)-like methods applied to approximately solve it have bad convergence properties.

We present in our talk a method of preconditioning which uses few iterations of a symmetric multigrid algorithm applied (at each (CG)-like iteration) to a system of which matrix is the Gram matrix of the finite element basis functions.

In the case of classical (CG) method applied to the normal equations associated to the initial system (if it is nonsymmetric),we prove that if the spectral radius of the symmetric multigrid algorithm is independent on the mesh size of the discretization,then so is the step error reduction factor of the (CG) method,and we give an exact formula of it in terms of the above mentioned spectral radius.

Numerical examples are presented also for some other classes of (CG)-like methods (as e.g. (CGS) or (GMRES)) applied to convection — diffusion equations which model the chemical catalytic reactor.

Multiscale Discrete Optimization (Tutorial)

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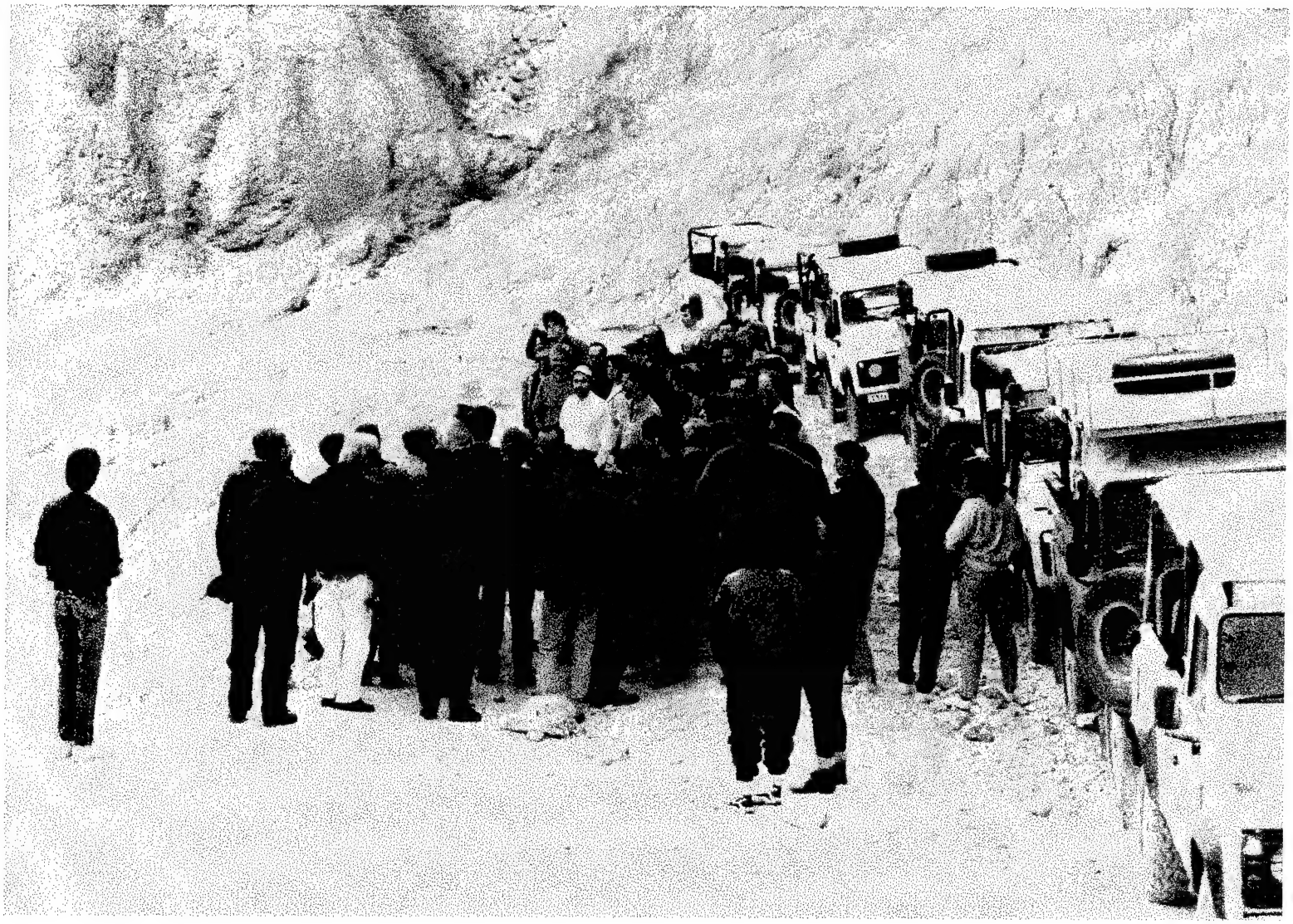
Abstract

The global minimum of functionals involving variables that may assume only discrete values (such as spins with only "up" and "down" states) is efficiently achieved by using multi-level interactions combined with "simulated annealing". Local minima are thus easily escaped.

Of special interest to physicists are the Ising model in a random field and spin glasses which are known to lead to difficulties in conventional Monte-Carlo algorithms, especially for low temperatures. These principles can also be applied to other optimization problems involving discrete-state variables such as the traveling salesman problem and molecular dynamics.

Light of science on multiscale landscapes



Pondering linear mechanical dynamics

Analyzing Electronic Circuits with Multi-Rate Signals Efficiently

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Abstract

Signals spanning widely-separated (or multi-rate) time scales arise in many important electronic circuit applications. Detailed analysis of such circuits, many of which are strongly nonlinear, is often difficult or impossible using existing analytical or computer-aided methods. In this work, an analytical formulation and numerical methods are presented for analyzing strongly nonlinear circuits with multiple, widely-separated, time-scales of activity. The formulation uses multivariate functions to capture multi-rate behaviour efficiently, and the numerical methods solve a special hyperbolic partial differential equation to obtain these multivariate functions. The formulation and numerical techniques are both in the time domain, which enables the approach to analyze strongly nonlinear circuits accurately and efficiently. The numerical methods scale linearly with circuit size, hence are practical for large circuits; moreover, the effort required is independent of the values of the multiple rates. Results are presented for several strongly nonlinear multi-rate examples.

Abrupt Learning and Retinal Size Specificity in Illusory Contour Perception

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Abstract

The distinction between gradual and abrupt improvement in performance is commonly made in behavioral studies of learning. Perceptual learning is often characterized by gradual, incremental improvement, and is found not to generalize over stimulus manipulations such as change in retinal size or location. Consequently, it has been suggested to involve synaptic modifications in early cortical areas. In contrast, an abrupt improvement in performance, such as when observers suddenly see the camouflaged Dalmatian dog, is usually taken to indicate a cognitive event ("insight") which occurs more centrally.

I will describe experiments on illusory-contour perception where subjects undergo an abrupt perceptual transition, resembling an incident of insight. The transition is triggered by specific visual stimuli, and leads to an abrupt improvement in psychophysical performance. Surprisingly, the learning is found not to generalize to a new retinal size, and re-training is necessary. These results suggest that the two forms of learning may share a common mechanism — a proposal made by Hebb (1949) almost half a century ago.

Algebraic Multigrid Methods (AMG): A Tutorial

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Abstract

Multigrid methods have proved to be very effective in the solution of many types of problems. The key to their success is that single-grid relaxation methods (e.g., Gauss-Seidel), while generally poor solvers, are very efficient smoothers (that is, error is smoothed quickly). This smoothed error can be well approximated by interpolation from a coarser mesh, and a coarse grid equation for this error can be formulated and solved, with the interpolated solution used to correct the finer grid approximation. A recursive application of this process ("solving" the coarser level problem again by relaxation and appeal to still coarser grids) yields a multigrid "cycle", which reduces overall error by a small factor (0.25 is typical) independent of the size of the fine grid and in an amount of work equivalent to just a few fine grid relaxation sweeps.

The majority of work has been done using logically rectangular meshes, which allows for uniform coarsening and application of multilevel solution methods in a (relatively) straightforward way. At times, application of usual multigrid methods is not practical (or even possible). Of particular interest are problems discretized on unstructured grids, often used with irregular, complicated domains and using local refinement. Other examples are problems with highly varying or discontinuous problem coefficients, and even purely discrete problems.

Algebraic multigrid was developed in order to handle such problems. An algebraic interpretation of smoothing by relaxation can be inferred from the operator alone, which allows an automatic choice of the coarser levels, interpolation, and coarser grid operators. With these defined, usual multigrid cycles can be performed. This introductory AMG talk motivates and describes the basic AMG algorithm, and results are presented for a number of model problems. In addition, limitations of the basic algorithm and extension of this algorithm to different problems (such as discretized systems of PDEs) will be discussed.

Time Scales and Nonstationarity in Complex Systems and Applications to Epilepsy

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Abstract

Distinguishing between the effects of nonlinearity and the effects of time dependent dynamics in complex systems is a very difficult problem. We present a new method for approaching this problem. The method is based in using information theoretic measures to characterize the dynamical distance between windows of a time series. If the dynamical distance is large, that is evidence that the underlying dynamical system generating the data is time dependent. We show how to construct a geometric representation of this time dependence in a "meta-phase space". The geometry in this meta-phase space characterizes certain features of the time dependence of the dynamics. We show how the method can be used in applications to 1. a mechanical problem of a shaft rotating in a ball bearing sleeve, and 2. an analysis of data collected from depth electrodes of patients with temporal lobe epilepsy. The nature of the meta-phase space construction is dependent on the time scales over which the system is analyzed.

Adaptive Wavelet Methods for Nonlinear PDEs with Applications to Navier–Stokes and Reaction–Diffusion Equations

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Abstract

The talk is focused on adaptive wavelet methods for the numerical solution of evolutionary PDEs. The developed method is based on the concept of multiresolution analysis and the use of operator–adapted biorthogonal wavelets in a Galerkin–type approximation. We construct fast adaptive transform algorithms ($O(N)$) for the decomposition of a function into a lacunary wavelet basis, i.e. a basis constituted of a subset of all basis functions up to a certain scale, without modification. The approach is based on the explicit computation of scalewise contributions of the approximated function to the values at points of hierarchical grids.

Adaptive reconstruction algorithms for sparse wavelet series on irregular grids are also presented. The construction employs the cardinal function of the multiresolution. The algorithms for the one and two–dimensional case are described in detail, higher dimensions are straight forward.

The new method is applied the solution of nonlinear parabolic PDEs with semi–implicit discretization in time and self–adaptive wavelet discretization in space.

Applications are concerned with reaction–diffusion equations. Results with full adaptivity of the spatial wavelet discretization are presented for one–dimensional flame fronts as well as for two–dimensional problems. The numerical simulation of two–dimensional flame balls exhibits the thermo–diffusive instability, observed in the experiments and predicted by the theory.

Furthermore, the method has been applied for the numerical simulation of two–dimensional homogeneous decaying turbulence and to the interaction of three vortices. The main motivation comes from the fact that turbulent flows, dominated by coherent structures, have a sparse representation in wavelet bases. Up to now, wavelets have been used only for analysis or compression of turbulent fields, calculated by other classical methods. Here we solve the Navier-Stokes equations

directly in an orthogonal wavelet bases and demonstrate the possibility to benefit from the compression property of this representation.

From comparison of the results with those calculated by a classical Fourier pseudo–spectral method we can deduce that the deterministic predictability is retained with a reduced number of degrees of freedom. In the conclusion we discuss some perspectives for turbulence modeling in the wavelet-coefficient space.

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Multi-Scale Low-Level Visual Representation and Fast Processes

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Abstract

A fast multi-scale low-level representation of an image is introduced followed by a general framework for fast curve completion (over gaps) processes in all different scales. The importance of a multi-scale definition of completion fields, with specific relations between scales of length, width and curvature, is pointed out. Based on these a fast segmentation process is outlined. Specifically, a fast numerical method for computing the curve of least energy (elastica) and its energy will be introduced. Moreover, two novel simple analytic approximations to the curve of least energy will be presented, together with simple expressions for their energies.

Interfacing Models: Polyethylene

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Abstract

A single polymer chain of a high degree of polymerization is an object extending over 3 orders of magnitude of spatial length scales (bond length, 1Åto radius of gyration, 1000Å). To these length scales there corresponds an even broader extend of time scales, from 10^{-15} seconds for bond length vibrations up to 1 second for a complete renewal of the chain conformation. To simulate such a system, no single model — with its fixed intrinsic length and time scale — will suffice.

We will present results obtained on 4 distinct levels of models applied to polyethylene (PE), which can be regarded as the fruit fly for polymer modelling. Starting from an ab initio quantum chemical calculations on the chemical building blocks of this polymer, we proceed to parametrize force fields for a classical Molecular Dynamics (MD) simulation using a fully atomistic description of the chain. We will show results on static and small time dynamic properties of alkane chain melts (short PE chains) obtained with this model and compared to experiment.

On a slightly more abstract level of description, one carbon atom with its attached hydrogen atoms is treated as a single united atom, thereby reducing the number of force centers in the system, enabling us to perform simulations on larger length and time scales. We will show results on the large scale dynamics of alkane chains and compare to experimental data.

In a final step of abstraction, we map the chemically detailed models used so far to a lattice model (bond fluctuation model) which is simulated via a Monte Carlo (MC) procedure. In this step we employ the universality found in the description of polymers on large length and time scales, which enables a treatment of these scales with very abstract models, and try to determine the non-universal prefactors occuring in the universal laws by input information from the detailed models on the smaller scales.

Why the Hell am I Here?

Sorin Solomon
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Abstract

The talk was conceived as an informal opening address. It served as a quick orientation and working guide by:

- exposing the main motivations of the meeting,
- introducing the various components of the attendance one to another,
- sketching the conceptual structure of the meeting,
- explaining the self-organizing mechanisms of talk initiation and talk scheduling.

It also stressed the role of the multiscale paradigm as a coherence factor between the very wide range of subjects and fields represented at the meeting.

Creativity and Multilevel Connectionism

John Spinks

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Abstract

Creativity is one of the more difficult areas to study psychologically, as exemplified by the problems we have in defining the concept or the processes involved. It can be studied at one or more of many levels of explanation and description, and a brief summary of some of the main factors which are related to changes in creative productivity will be presented. The talk will then go on to describe an alternative view to describing creativity, by using the concepts of semantic space, neural nets and connectionist perspectives. Such approaches can be modeled on computers, and, in the process, a deeper understanding of the mechanisms involved may emerge. The talk will also look at the roles of awareness and consciousness in the creative process, and how these might be mapped onto current perspectives of brain processes.

Sex and the Single Bit

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Abstract

The Penna model of biological ageing was generalized by de Oliveira to include sexual reproduction. Like energy versus entropy, it is based on a counterplay of Darwinistic selection of the fittest versus random new mutations most of which are bad. The sexual variant allows to discuss questions like: Are men faulty products of nature? Why do women live longer than men? Is sexual cannibalism the answer?

Multiscale Relaxation of Ising Models

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Abstract

Simulations on 256 nodes of a Cray-T3E confirmed that the magnetization of the Ising model relaxes to its equilibrium value with a *stretched* exponential below the critical temperature in two dimensions, but with a simple exponential above Tc and/or in higher dimensions. Proper multi-scale dynamics of Becker-Doring cluster growth gives this result, while simple superposition of independent exponential decays for different cluster sizes would be wrong. Spin-spin autocorrelations in equilibrium are not an appropriate tool for this stretched-exponential question.

One-Shot Methods for Differential Optimization

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Abstract

We discuss the efficient multigrid solvers for optimization problems governed by partial differential equations, with emphasize on boundary control and shape optimization problems. The adjoint method is used for fast calculation of gradients. Moreover, it is shown that for proper coarsening one must introduce adjoint variables (Lagrange multipliers). For small dimensional design space the update of the design variables is done only on the coarsest grids, while as the dimensionality of the design space increases more grids are involved in the optimization iteration. For the infinite dimensional case, all grids are used to update the design variables. A general theory for the design of smoothers for optimization problems is explained, and its use in some model problems is demonstrated. In general, the gradient direction does not provide the desired smoothing property. Preconditioners for optimization problems for the infinite dimensional design space are constructed using pseudo-differential calculus. They allow efficient solvers in which the optimization is 'outside' the multigrid solver for the constraints. Example from fluid dynamics including the full potential equations and the Euler equations are given.

Issues in Computational Fluid Dynamics

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Abstract

Efficient solvers for the equation of fluid dynamics are discussed. We focus on the main obstacles on reaching optimal multigrid efficiency for real flows. We distinguish between difficulties arising from different sources. This include the mixture of elliptic and hyperbolic parts in the equation, the limitation of non-directional relaxation in converging characteristic components for hyperbolic problems, the necessity of using marching techniques for hyperbolic parts, h-elliptic discretization for the elliptic parts, and upwind biased for the hyperbolic ones. Issues related to anisotropy in relation to discretization and to the partial differential equation are mentioned and possible solution strategies are examined. Examples of a few discretizations which obey the desired properties are shown for the compressible inviscid case in two dimensions. Results for exterior and interior flow cases are mentioned.

Basic Multigrid Tutorial

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Abstract

In the first lecture the fundamental multigrid idea (smoothing and coarse grid correction) and the basic multigrid algorithms (MGI and FMG) are described. Some additional remarks are made with respect to multigrid literature. The tutorial is structured as follows:

(0) General remarks

(1) Multigrid idea, smoothing

(2) Two-grid cycle

(3) Multigrid cycle (MGI)

(4) Full multigrid (FMG)

In an additional lecture the following topics are mentioned

(5) Nonlinear multigrid (FAS)

(6) Anisotropic equations

(7) Parallel multigrid

(8) Adaptive multigrid

Some Main Principles of Computer Modelling and Simulation System Development

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Abstract

Some main principals of general theoretical approach to creation and development of computer modelling and simulation system for multiscale phenomena research will be considered. Some information on the realization of such approach ("Interactions" System) and an example of investigation of living cell biochemical mechanisms, its interactions with anti cancer drugs will be given as an illustration.

1. What and why: difficulties, reasons:

1.1. Multiscale systems
(multidisciplinary; multilevel — scales of generalization, time-scales).

Difficulties:

(a) Long-lasting, non sufficient productive formalization processes.
Reason: de-coherence of the descriptions with large dimensions and high complexity.

(b) De-coherence.
Reason: difference between the implementing languages (base concepts, semantics, syntax).

(c) Formalization, and computer formalization.
Reason: non-adequacy, non sufficient adequacy of basic concepts of implementing formalized languages.

1.2. Computer modelling and simulation system (CMS) implementations: investigation, design, control.

Difficulties:

Organization of integration activity of participants.
Reason: different languages of participants, different deductive means, non-productive deductive system as a whole.

1.3. Aims, ways and some main principles of CMS development.

Aims: increase productivity and efficiency of creation of 1.2.
Ways: elimination of difficulties of 1.1. and 1.2.
Main principles: creation of common conceptual base, language and deductive means for interdisciplinary activity.

2. **Tasks**:

(1) Creation of the conceptual basis of the scientific knowledge system language.

(2) Creation and development of computer language for (1).

(3) Verification (1) and development of computer system on the base of (2).

3. **Conceptual basis of the scientific knowledge system language**:

3.1. Scientific knowledge system:

(a) Subject area: knowledge is presented in the form of laws of functioning of physical phenomena.

(b) Formal methodological area, common for all subject areas: knowledge is presented in form of general methods applicable to the description and analysis of diverse laws.

Concepts, languages, and methods of (a) and (b), that exist as a common arsenal, represent and satisfy the researches needs only partially:

(1) Interrelations between such notions as "space", "time", and "substance", "substance localization (its states and changes in time and space)" requires a comprehensive analysis of these notions in order to be able to introduce methods of the description of irreversibility and specifics of the physical reality reflected in the statement of the second principle of thermodynamics.

(2) The methods of laws description do not include any common methods and tools for the description of experimental facts, relations and properties of specific objects as parts of a whole, the available mathematical languages are not oriented toward expressing the differences between relations and those objects on which the relations are realized.

(3) The information contained in the subject area of the knowledge system is given in terms of different specialists and at different semantic levels; the relations between these levels are the relations between the concepts of different disciplines interlinked with these levels.

3.2. The key notions of the conceptual basis of the language:

The key notion of the conceptual bases is an experimental fact, its description revealing the elementary property of a material object under certain conditions of the reality.

The properties of a material object presented through the description of the laws and their manifestation define the object along with the laws which determine the probability of manifestation of the object's properties at certain instants of the object's lifetime.

The variation of this probability (a decreasing function P(lifetime), depending on the object's lifetime) is an irreversible process — provided the object structure remains unchanged — depending on the history of exist of the object and its previously manifested properties.

3.3. Base syntactic construction of language: A propositional form — the frame for describing the properties of the object — is taken as a major unit of language. The frame is intended to provide the description of fundamental abstract objects of the empirical — phenomenological relations.

4. **Deductive system as a whole:**

Languages, abstract (different levels) and concrete definitions of reality, inference.

5. **Description and investigation of manifestation of the large scale system properties:**

5.1. Description of complex phenomena:

The description of cause-effect relations between these frames forms a certain net of interrelated objects in compliance with the logic of events taking place in the changing world.

The description of events — changes of the object states in time — together with the logical conditions which determine manifestation of certain qualities is the description of localization of the occurrence of physical processes in system of interrelated objects.

The introduction of P functions for each individual object (and the system as a whole) is the introduction of a way to describe irreversibility corresponding to the second principle of thermodynamics.

Such a description allows one to relate the description of manifestation of the system properties with the description of manifestation of properties of its individual elements and takes the meaning of the concepts (terms) — phenomenological higher level descriptions of laws of phenomena —

comprehensible in terms of compositions of phenomenological lower level descriptions of phenomena.

It takes it possible to give a logical formal presentation of information in the knowledge system provided by different subject disciplines.

5.2. Representation of 3.1: (1), (2), and (3).

6. **Computer modelling and simulation system creation.**

7. **Results:**

7.1. Verification of the main hypotheses.

7.2. Ways of development.

7.3. International projects.

Description and Investigation of Biochemical Mechanisms of Living Cell

Co-lecture with:

Some Main Principles of Computer Modelling and Simulation system Development

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Abstract

Some main specifics of multiscale modelling and computation processes are illustrated by a concrete example: investigation of biochemical mechanisms of living cell, its interactions with anti cancer drugs.

Aims: Effective chemotherapy schemes creation.

1. **Multiscale description of phenomena**:
   - 1.1. Enzyme reaction as a complex system.
   - 1.2. Phenomenon of enzyme reaction as a whole.
   - 1.3. Biochemical mechanisms of living cell as a complex heterogeneous system of large amount of enzyme reaction interactions.
   - 1.4. Cause-effect relations and dynamics of processes.
   - 1.5. Interactions with drugs.
   - 1.6. Measurement procedures.
2. **Modelling and computation**:
   - 2.1. Data bases: metabolic pathways, enzymes, metabolites, general physic-chemical laws, kinetic parameters, experimental data.
   - 2.2. Automatic generation of computer models.
   - 2.3. Computation, identification, investigations.
3. **Research cycle as a whole and results.**

Information:

System of mathematical methods for computer modelling and simulation

"Interactions"

The System is intended for the design and study of mathematical computer models of *large scale* phenomena in different areas of science and technology.

The System is applicable to computer-aided design, scientific research, planning and control.

The development of the system means and techniques is aimed at an *increase of productivity* and *efficiency* of formulation and analysis of scientific hypotheses, design and plan solutions, management actions, etc.

The Language of System is oriented to the description of phenomena laws in theoretical and empirical terms and is based on the system of notions and concepts which allows the design and investigation of models of *different scales* and *dimensions* constructed at different semantic levels, and the provision of common semantic and technological basis for various applications, i.e. for designing the problem-oriented and dedicated languages.

The *Language* is formulated as that of a general theory whose basic concepts are intended to facilitate the description of complex physical phenomena and system elements through the description of their properties, i.e. operation laws, description of the environment conditions, interaction of elements, structure of the system, and experiments carried out with the elements and the system in its entirety.

The major syntactic unit of the language is the frame for the element's properties description which contains different kinds of variables and statements, and allows easily to describe cause-effect relations between events and complex dynamical processes in system.

The System allows the design of models consisting of descriptions of separate subsystems with the use of multilevel hierarchical definitions, both specific and general definitions for classes of diverse semantic levels employing sets of elements or subsystems as their variables.

The language of the System interprets the notions of widely used mathematical disciplines: the theories of algorithms, differential (difference) equations, random processes, various kinds of net models, finite-state machine theory, reliability and queueing theories, and some others.

Problem oriented and dedicated languages, vocabularies and model thesauruses are designed with the help of systems of multilevel definitions of concepts and different libraries of the System.

Vocabularies and model thesauruses are complex descriptions of diverse phenomena (as a whole, and its parts) which accumulate the knowledge of different specialists, interpreted in the common base language.

The System is complete with simulation organization means and debug means.

Software means of the System contain the mobile facilities for its application (through the adaptation in current revision) with different types of computers and are a high level operation system functioning in combination with implemented computers.

The current Computer version "Interactions 96" is based on the JAVA. Now Java-based version is in progress, and this version will be supported in future.

The software set is also oriented to its use in multiprocessor and multicomputer systems.

The System is used to solve problems in different areas of scientific and practical activities.

Renormalized Quantum Field Theory from Renormalization Invariance

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Abstract

Renormalized quantum field theories can be represented as renormalized trajectories in the space of effective actions. We consider two basic examples, the Gross-Neveu trajectory as an example of a fermionic theory and the ϕ^4-trajectory as an example of a bosonic theory. We show that both renormalized trajectories are unique solutions to a renormalization problem of the following type: a curve which emerges from a renormalization fixed point, tangent to an eigenvector of the linearized flow at the fixed point, which is invariant up to a flow of a running coupling. The transformation law is shown to have a unique finite perturbative solution. No reference is made to a bare action. The role of reparametrizations of the running coupling and normal forms of the β-function are discussed.

Turbulence Simulation Using Sparse Grids

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Abstract

Direct numerical simulation of turbulent flows is very expensive because very fine grids and also very small time steps must be used to resolve the fine structures of 3-dimensional flows. This is true as for spectral methods as for FD or FE-methods. The sparse grid discretization in our experience can save about two orders of magnitude in storage requirement. In the neighbourhood of the boundary which plays an important role in the creation of turbulence the accuracy of our approximation is much better than in the case of standard grids.

References

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Sparse Grids

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Abstract

The sparse grid approach is a variant of the FE-method based on tensor products of hierarchical basis. The basis functions are selected from all possible product functions according to the contribution to the energy function which is to be minimized. This yields a straight forward adaptivity criterion. For good approximation properties only certain mixed derivatives are needed and for sufficiently smooth functions the computational complexity does not grow exponentially as it does for standard FE- or FD-methods.

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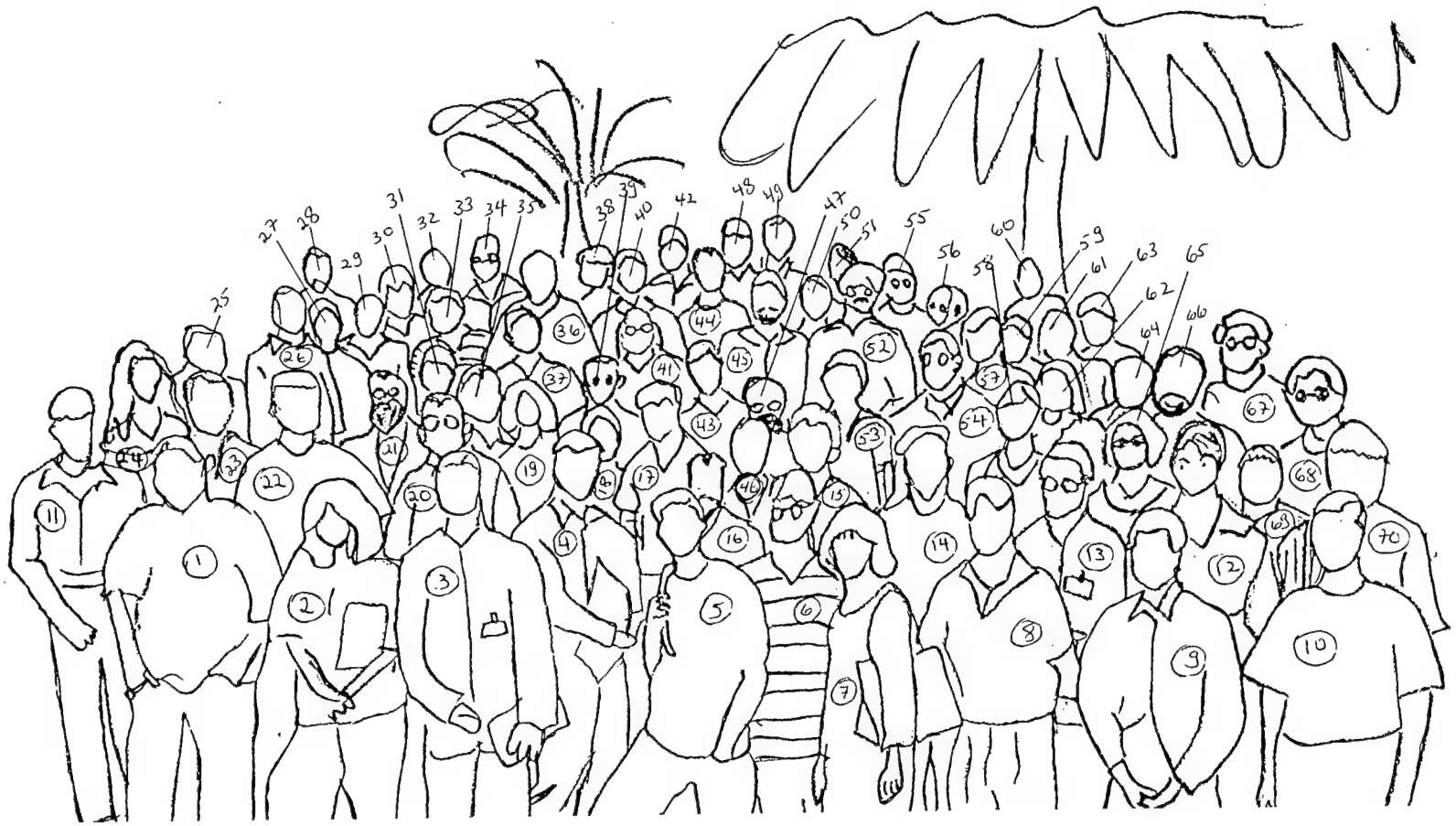

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Research Workshop of the Israel Science Foundation

Multiscale Phenomena, Modelling and Computation

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